

The Free Bose Gas with Flowing Condensate in Algebraic Quantum Field Theory

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*With love and gratitude
to my parents
Ingrid Hein, née Buddeberg,
and
Dr. med. Arnold Hein,
as well as to my grandparents
Irmengard and Heinrich Buddeberg,
who supported me generously*

Preface

*Spin & statistics
- and that's all*

We owe to F. LONDON the interesting idea that Bose-Einstein condensation underlies the superfluid behavior of matter. In fact, the condensation of the interaction-free Bose gas already shows some characteristic features from which many superfluid phenomena can be derived. Field theoretically, the long range order of the two-point correlations (off-diagonal long range order) is characteristic, and thermodynamically the entropy freedom of the condensate. Hydrodynamically, the equilibrium states of the Bose condensate are naturally described in TISZA'S two-fluid model. In particular, persistent flows of the condensate against the resting "normal" component emerge, and the velocity field of this flow is irrotational except for singularities with quantized circulation.

These properties enable us to qualitatively understand, and at least partially estimate quantitatively, a considerable range of experimental observations for helium II, such as critical densities and temperatures, the disappearance of the shear viscosity in the superfluid, the frictionless flow through capillaries and superleaks up to a critical speed, the thermomechanical effect, critical rotation phenomena and more.

It is thanks to the combined efforts of many researchers to develop a more rigorous, 'algebraic' basis for quantum field theory and its application to statistical mechanics, that the equilibrium states of the free Bose gas can now be classified relatively completely. In the presence of condensate, they exhibit all the field-theoretical and thermodynamic features cited above. We will prove that the thermodynamically pure phases are also characterized by the hydrodynamic properties mentioned. Most interestingly, these equilibrium states show persistent flow of the condensate with quantized vortices.

With the present constructive proof that such states exist within the solvable model of the interaction-free Bose gas, algebraic quantum field theory provides a solid new argument for the correctness of LONDON'S view. The characteristic behavior of a superfluid is essentially anchored in the Bose-Einstein statistics, that is, no special interaction is required for its basic qualitative understanding. The main goal of this work is to demonstrate this to the - admittedly incomplete - extent to which the aforementioned features characterize a superfluid. So if such a proof could be provided, we have attained our intended result.

It is hence be no means our aim to reproduce all the properties of helium II. In order to develop a further complete theory of superfluid helium on the basis of our investigations, it would first have to be clarified which are the condensing Bose particles that behave almost like interaction-free particles. If these are not the helium atoms themselves, but rather 'clusters' of atoms that combine into new elementary units (similar to Cooper pairs), then the superfluid component cannot of course simply be identified with the proportion of helium atoms in the ground state. The

known discrepancies between this proportion and the density of the superfluid suggest that such cluster formations do indeed occur within helium.

In summary, we do not want to and cannot give a complete description of all superfluid phenomena in terms of Bose-Einstein condensation. The free Bose gas represents a simple mathematical model that will prove to be far from perfect when measured against the real conditions in nature. As a mathematical model, it still has its justification in providing fundamental insights, such as the aforementioned scope of LONDON'S hypothesis. In contrast to the most precise possible computational reproduction or prediction of special measurements, structural modelling of nature in rigorous mathematical terms also has its own *raison d'être* simply for understanding fundamental, sometimes very abstract relationships, and in presenting them in an idealized manner.

Last but not least, maths has its own beauty, which hopefully remains tangible under the sequence of definitions, theorems and proofs that also formally underline the intent of this work as a coherent mathematical model for a fascinating physical phenomenon.

Aachen, in January 1979



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1. Introduction and overview

It is astonishing that in some quantum systems states of higher energy can be excited at low temperatures from which there is practically no dissipation. In nature, we encounter for example persistent currents and particle flow in superconductors and in helium-4 below the critical temperature. LONDON [1] was the first to connect the behavior of superfluid helium (helium 2 - He II) with the "condensation in momentum space" predicted by EINSTEIN [3] in 1924. Since then, this suspected connection and the question of how far it extends has been a subject of research. Progress in this direction is tied to advances in the statistical theory of quantum systems with infinite degrees of freedom, of which the Bose gas (already in a finite volume) represents one.

In the traditional formalism of quantum field theory the non-relativistic Bose gas is described by a scalar field $a(x)$ in $\mathbb{R}^3$, which together with its adjoint field $a^*(x)$ satisfy canonical commutation relations (CCR):

$$\begin{aligned} [a(x), a(y)] &= [a^*(x), a^*(y)] = 0 \\ [a(x), a^*(y)] &= \delta(x - y) \end{aligned} \quad (1.1)$$

The spatially homogeneous condensation of the free Bose gas into the ground state then leads to a class of translation-invariant equilibrium states with the two-point functions

$$\langle a^*(x) a(y) \rangle = |c|^2 + w(x - y) \quad , \quad (1.2)$$

where c is a complex order parameter and w is a rapidly decreasing rotational invariant real-valued function. These conditions and the associated representations of CCR were examined by ARAKI and WOODS [4]. CANNON [5] and LEWIS & PULE [6] generated these states in a volume limit.

In the two-liquid model, the two-point correlations (1.2) lead to a condensate with a spatially constant density $|c|$ that is completely at rest in relation to the normal liquid. Superfluid behavior in the form of persistent flow, on the other hand, requires a breaking of the Euclidean symmetry in the two-point function. In 1970, ROCCA, SIRUGUE & TESTARD [9] published a general measure-theoretic characterization of the equilibrium states of the free Bose system. It also covers states with symmetry breaking two-point functions of the form

$$\langle a^*(x) a(y) \rangle = \overline{Q(x)} Q(y) + w(x - y) \quad . \quad (1.3)$$

With a solution polynomial Q of the Laplace equation (i.e. a "Maxwell polynomial"), they describe the particle correlations of the thermodynamically pure phases of the Bose condensate.

The generation of such symmetry breaking states in the thermodynamic limit and in particular the boundary conditions under which they arise, e.g. as limit states of

Gibbs ensembles, could provide information about their formation mechanisms. ROBINSON [10], for example, discusses the idea of phase separation in the Bose system as a result of the binding of certain single particle states to an attractive surface potential. The possibilities of describing such potentials through boundary conditions for the one-particle Hamiltonian or by means of a modified chemical potential can be used to create specific equilibrium states. Another path that can be followed - again for the creation of special states - leads via a volume limit with the rotating vessel of BLATT & BUTLER [12]. The symmetry breaking thermodynamically pure phases can be generated using BOGOLIUBOV's method of "quasi-averages" [48]. This approach does not have as intuitive a physical interpretation as the other two methods, but allows states to be created with an arbitrary Maxwell polynomial Q in the two-point function (1.3).

Of course, the physical properties of these states themselves are of primary interest - precisely in view to further elucidating the connection between superfluidity and Bose condensation. In order to simulate certain properties of helium II in the Bose condensate, ONSAGER & PENROSE [13] ad hoc postulated the general form $\overline{q(x)} q(y)$ for the particle correlation in the condensate, as early as 1956. In fact, a term of this form - largely independent of special properties of the function q - leads to a generally non-vanishing particle flow and a canonical hydrodynamic velocity field $\mathbf{v}_s$. In an equilibrium state, $\mathbf{v}_s$ appears as a persistent superflow. Moreover, $\mathbf{v}_s$ is irrotational, except for singularities with quantized circulation and thus reflects the experimental findings of "metastable" quantized vortices in helium II, cf. VINEN [14] (later also WHITMORE & ZIMMERMANN [15]). Also, a staircase-like increase in the vortex strength of the very slowly rotating helium II was observed by PACKARD & SANDERS [16]. This finds an explanation in abrupt phase transitions between different vortex states of the Bose system at critical asymptotic surface velocities of rotation.

In statistical mechanics, the need to consider infinite systems arises from the well-known fact that phase transitions do not occur in finite systems (the state functions here generally behave analytically, cf. GRIFFITH [17]). However, the Fock space is unsuitable for the description of infinitely extended statistical quantum systems because it does not contain any states of non-vanishing average particle density. The equilibrium states we examined are not normal states in Fock space. However, for each state there exists a representation of the canonical commutation relations in which this state appears as a Hilbert space vector. In order not to exclude any physically interesting representations from among all the inequivalent representations of the CCR (or also of the canonical anticommutation relations, CAR) in systems with infinitely many degrees of freedom, algebraic QFT describes the system from the outset using a universal C^* -algebra. The states are represented by positive normalized (hence continuous) linear functionals on this algebra [18, 19]. Only after choosing a specific representation do field operators have a well-defined meaning as operators in a Hilbert space. Among all representations of a C^* -algebra, each state distinguishes a canonical *cyclic* representation. The self-adjoint elements in the operator algebra of any representation provide the observables of the proposition lattice in which the physical system is logically described.

In Chapter 3 the Weyl algebra is first defined as the universal CCR C^* -algebra. Instead of starting directly from the canonical commutation relations, we take a detour via the Weyl relations, which are technically easier to handle.

As is well known, a more rigorous analysis of the canonical commutation relations (1.1) shows that the fields a and a^* have to be regarded as operator-valued distributions. Only their connection ("smearing out") with suitable test functions leads to well-defined operators in a Hilbert space $\mathcal{H}$.

For test functions u, v we write these field operators

$$\begin{aligned} a(u) &= \int_{\mathbb{R}} a(x) \overline{u(x)} dx \\ a^*(v) &= \int_{\mathbb{R}} a^*(x) v(x) dx \quad . \end{aligned}$$

The CCR are now written more precisely in the form

$$[a(u), a^*(v)] \subseteq \langle u, v \rangle Id_{\mathcal{H}} \quad . \quad (1.4)$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product in $L^2(\mathbb{R}^3)$ and $\subseteq$ indicates that the two sides of (1.4) agree on a dense subset of $\mathcal{H}$. The relation (1.4) can only be realized with unbounded operators $a(u)$ and $a^*(v)$, i.e. operators that are at most densely defined in $\mathcal{H}$. However, some of the technical difficulties caused by this can be elegantly circumvented by rewriting the CCR in the form of the slightly stronger Weyl relations

$$w(u+v) = e^{\frac{1}{2}Im\langle u, v \rangle} w(u) w(v) \quad . \quad (1.5)$$

Therein is $w(u) := \exp(\frac{1}{2}(a(u) + a^*(u)))$. Using common techniques, the canonical commutation relations (1.4) can then be recovered from equation (1.5) (cf. SEGAL, [20], p. 15 ff.).

The equilibrium states of the free dynamics of the Bose gas will be classified in Chapter 2 independently of any special representation. We assume the Kubo-Martin-Schwinger (KMS) boundary condition, which provides an abstract analytical characterization of the thermodynamic equilibrium. It is known that it generally allows a variety of solutions for infinite dynamical systems. The physical meaning of all KMS states is not clear from the outset. However, HAAG, KASTLER & TRYCH-POHLMEYER [22] succeeded in an equivalent reformulation of the equilibrium conditions in purely physical terms. According to it, the extremal KMS states are characterized by a particular stability against local perturbations in the dynamics. In applying their stability criteria to the states of the free Bose gas, in 1977, HAAG & TRYCH-POHLMEYER [23] came across exactly the aforementioned class of states with a two-point function (1.3), where Q denotes a solution polynomial of the Laplace equation.

We will examine the role of the Laplace equation in still more detail. ONSAGER & PENROSE [13] referred to the function Q , which determines the order parameter of the condensate, as the "wave function" of the condensed Bose particles. This naming is somewhat unfortunate and may have contributed to the fact that it was not possible to find corresponding states for so long. In Chapter 3 it becomes clear that the Laplace equation does not appear here as a Schrödinger equation. As a result, we have to consider Q not as a wave function, but rather as a classical field.

There is therefore no need to require normalization for Q (which was already not the case in (1.2)). Furthermore, it is not at all suprising that functions Q and cQ with any $|c| \neq 1$ belong to different states.

In Chapter 4 it is shown that states with a two-point function (1.3) have a characteristic hydrodynamics. The terms “quantized vortex”, “vortex strength”, “vortex core”, etc. are clarified and illustrated using a small collection of examples. Typical vortices of the Bose condensate are straight lined or circularly closed. In the latter case, they allow the interpretation as rotons, in the sense of FEYNMAN [24], who discussed similar vortex phenomena in superfluid helium (ibid, p.330). In the Bose condensate, the vortex quantization finds its simple formal explanation in the special shape of the closed differential form assigned to the hydrodynamic field $\mathbf{v}_s$. Far beyond the scope set here, the formal occurrence of comparable phenomena, such as those discussed for example in superconductors of the second kind or in quark confinement, is of some general interest. Chapter 5 is reserved for the creation of these states. The purpose of the thermodynamic limit is not only to provide information about possible mechanisms for the formation of special states. It is also to establish the relationship to classical thermodynamics. The thermodynamic state functions (entropy density, pressure, etc.) do not represent local observables in the field theoretical sense. They can often only be derived in a volume limit from the corresponding state functions of finite Gibbs ensembles, be it directly or via extrapolated state equations. Either way, it turns out that the thermodynamics of the condensed component is trivial in the sense that the latter does not contribute to entropy or pressure. So at this point, the “new” states behave exactly like the known “old” ones with a translation invariant condensate. We show this in Chapter 6 using the states generated in Section 5.1.

The question remains as to how the investigated KMS states arise from a non-equilibrium situation. For very special initial states in which only the superfluid component is locally disturbed, the return to equilibrium can still be derived from a field equation that is analogous to the time-dependent Schrödinger equation

$$\frac{\partial}{\partial t} Q = \frac{i}{2} \Delta Q \quad , \quad (1.6)$$

for $Q = Q(x, t)$. The well-known dispersion of wave packets then immediately causes the density of the condensate

$$\rho_s = \overline{Q} Q$$

to smooth down over time to the density of the original KMS state, if the latter is only locally disturbed. So if the perturbed state is $Q^\sim = Q + \psi$ with the Maxwell polynomial Q describing the condensate of the original unperturbed state and ψ any smooth function, such that $\psi(x, t) \in \mathcal{D}(\mathbb{R}^3)$ for all $t \in \mathbb{R}$, then substituting $Q^\sim$ into equation (1.6) immediately leads to

$$\frac{\partial}{\partial t} \psi = \frac{i}{2} \Delta \psi \quad . \quad (1.7)$$

The well-known spreading out of the wave packet ψ according to this equation now leads to the asymptotic return from $Q^\sim$ to Q for t towards infinity.

If we also allow non-local perturbations, this is equivalent to renouncing on any boundary conditions for the solutions Q of equation (1.6). However, these then generally no longer behave asymptotically in a time-stationary manner. Still further we are away from a general solution to the problem of transition to the equilibrium states presented here.

In the interest of a clear, concise presentation, we use a measurement system in which the mass of the Bose particles, Planck's constant and Boltzmann's constant are normalized to 1.

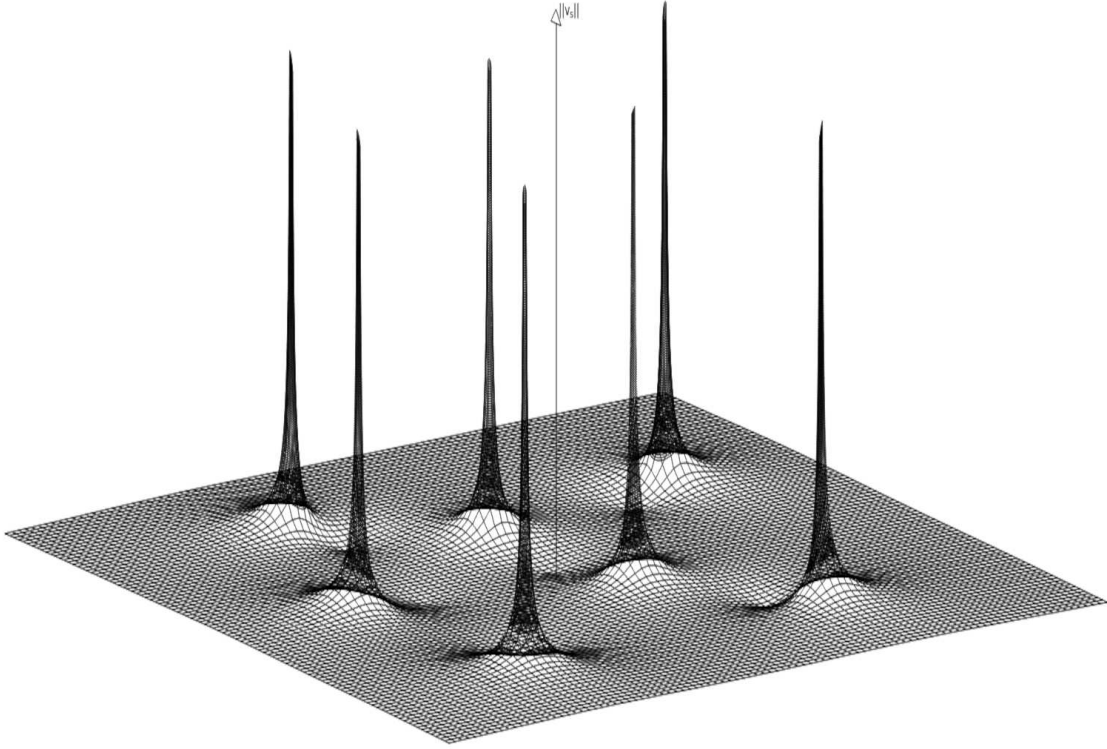


Fig. 1. Vortices in horizontal superflow. The flow velocity is displayed vertically.
Flow vectors see page 40, Fig. 4, holomorphic case.

2. Basics of the CCR Algebra

2.1. The Weyl Algebra

For any $\mathbb{C}$ -linear space $\mathcal{L}$ with non-degenerate real symplectic form $\sigma : \mathcal{L} \times \mathcal{L} \rightarrow \mathbb{R}$ and $\mathfrak{A}$ any C^* -algebra with unit $\mathbf{1}_{\mathfrak{A}}$ (the identity element in $\mathfrak{A}$), a mapping $w : \mathcal{L} \rightarrow \mathfrak{A}$ is called a *Weyl*system over $\mathcal{L}$ in $\mathfrak{A}$* , if and only if w satisfies the following three conditions.

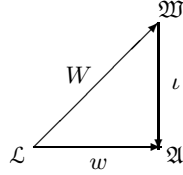
For every $u \in \mathcal{L}$ holds

$$(UN) \quad w^* w = w w^* = \mathbf{1}_{\mathfrak{A}} \quad , \quad \text{i.e. } w(u) \text{ is unitary in } \mathfrak{A} ,$$

$$(WR) \quad w(u+v) = e^{i\sigma(u,v)} w(u) w(v) \quad ,$$

and if $w : \mathcal{L} \rightarrow \mathfrak{A}$ is continuous on all finite-dimensional subspaces of $\mathcal{L}$ with respect to at least one W^* topology on $\mathfrak{A}$ induced by a faithful representation.

Definition The universal element $(\mathfrak{W}, W)$ of all Weyl*systems over $\mathcal{L}$ in the sense of the following commutative diagram is called the *Weyl algebra over $\mathcal{L}$* .



In words: For every Weyl*system w over $\mathcal{L}$ in $\mathfrak{A}$ there exists exactly one $*$ homomorphism ι from $\mathfrak{W}$ into $\mathfrak{A}$ such that $w = \iota \circ W$.

A construction of the Weyl algebra can be found, for example, in MANUCEAU [26]; see also SLAWNY [27], and in particular EMCH [28], p. 238, where Theorem 3.1.3 contains the universality property.

Following common usage, the Weyl algebra over $\mathcal{L}$ is henceforth written as $\mathfrak{W}(\mathcal{L})$.

Definition Every non-degenerate representation π of $\mathfrak{W}(\mathcal{L})$ such that $\pi \circ W$ is continuous on all rays of $\mathcal{L}$ in the Weyl*topology is called a *Weyl system over $\mathcal{L}$* .¹

If $\mathcal{L}$ is in the canonical way a linear submanifold of a Hilbert space $\mathcal{H}$ (for example $\mathcal{L} = \mathcal{D}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$), then $\mathcal{L}$ has the natural structure of a *prehilbert space* and we consider usually without explicit reference σ to be the following symplectic form (2.1.1) induced by the scalar product $\langle \cdot, \cdot \rangle$ in $\mathcal{H}$.

¹ Any representation π of $\mathfrak{A}$ in the algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators of a Hilbert space $\mathcal{H}$ is called *non-degenerate*, if and only if the range of π is dense in $\mathcal{H}$.
(Don't confuse a *Weyl system* with the previously defined *Weyl*system*.)

The canonical symplectic form in $\mathcal{L} \subset \mathcal{H}$ is

$$\sigma(u, v) = \frac{1}{2} \operatorname{Im} \langle u, v \rangle, \quad \text{for all } u, v \in \mathcal{L}. \quad (2.1.1)$$

Convention For $\mathcal{L} = \mathcal{S}(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$, the space of rapidly decreasing complex-valued C^∞ functions with canonical symplectic form $\sigma(u, v) = \frac{1}{2} \operatorname{Im} \langle u, v \rangle$, $\mathfrak{W}(\mathcal{L})$ is called the *tempered Weyl algebra*.

2.2. States

Definition Let $\mathfrak{A}$ be a C^* -algebra with unit $1_{\mathfrak{A}}$, for example $\mathfrak{A} = \mathfrak{W}(\mathcal{L})$. Every positive linear functional ω on $\mathfrak{A}$ such that $\omega(1_{\mathfrak{A}}) = 1$ is called a *state* of $\mathfrak{A}$.

A famous result by GELFAND and NAIMARK [30] and SEGAL [31] ensures that for each state ω on $\mathfrak{W}(\mathcal{L})$ there exists a (up to unitary isomorphism unique) *cyclic* representation π of $\mathfrak{W}(\mathcal{L})$ in the algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators of a Hilbert space $\mathcal{H}$, such that with a cyclic vector $\Omega \in \mathcal{H}$ holds:

$$\omega(A) = \langle \Omega, \pi(A) \Omega \rangle, \quad \text{for every } A \in \mathfrak{W}(\mathcal{L}).$$

This representation is called the *Gelfand-Naimark-Segal* (GNS) representation pertaining to ω . The classical construction of the GNS representation is also found in EMCH [28].

Definition For every state ω on $\mathfrak{W}(\mathcal{L})$, the functional E on $\mathcal{L}$

$$E := \omega \circ W$$

is called the *generating functional* (synonymously *characteristic functional*) of the state ω .

E is characterized by the following 'positivity property', which applies to all finite sequences $(\lambda_\nu, u_\nu)_{\nu=1}^n$, with $\lambda_\nu \in \mathbb{C}$ and $u_\nu \in \mathcal{L}$:

$$0 \leq \sum_{\mu, \nu=1}^n \lambda_\mu \bar{\lambda}_\nu E(u_\mu - u_\nu) \exp(i \sigma(u_\mu, u_\nu)) \quad (*)$$

Conversely, every functional $E : \mathcal{L} \mapsto \mathbb{C}$ continuous on rays with the property $(*)$ and additionally $E(0) = 1$ is the generating functional of exactly one *regular* state ω on $\mathfrak{W}(\mathcal{L})$, that is, the associated GNS representation is even a Weyl system over $\mathcal{L}$ (see for example [28], p. 239, Theorem 8).

Many properties of states of the '*local*' Weyl algebra over $\mathcal{L} = \mathcal{D}(\mathbb{R}^3)$, the space of complex valued C^∞ functions with compact support on $\mathbb{R}^3$, apply likewise to states of the tempered Weyl algebra over $\mathcal{S}(\mathbb{R}^3)$ due to the following lemma

Lemma 2.2.1. (ARAKI and WOODS)

Let $\mathcal{H}, \mathcal{K}$ be Hilbert spaces and $\mathcal{S}, \mathcal{T}$ separable topological $\mathbb{C}$ vector spaces with dense and continuous inclusions

$$\mathcal{S} \hookrightarrow \mathcal{T} \hookrightarrow \mathcal{H} \quad .$$

For every continuous generating functional E on $\mathcal{T}$, the cyclic representation π of the Weyl algebra $\mathfrak{W}(\mathcal{S})$ pertaining to $E \upharpoonright \mathcal{S}$ extends strong continuously in $\mathcal{B}(\mathcal{K})$ to the cyclic representation π of $\mathfrak{W}(\mathcal{T})$ for E in $\mathcal{K}$ and

$$[\pi \mathfrak{W}(\mathcal{T})]'' = [\pi \mathfrak{W}(\mathcal{S})]'' \quad ,$$

where $[A]''$ denotes the *bicommutant* of any set $A \subset \mathcal{B}(\mathcal{K})$; cf. [19], p. 48.

Proof: Everything follows from Lemma 2.3. in [4]: Due to the continuity of E and of the inclusions, and because of the density statements, there exists for every $u \in \mathcal{T}$ a sequence $(u_n)_{n \in \mathbb{N}} \in \mathcal{S}^{\mathbb{N}}$ which in $\mathcal{T}$ converges to u and thus also in $\mathcal{H}$, and

$$\lim_{m,n \rightarrow \infty} E(u_m - u_n) = 0 \quad .$$

Therefore, the cyclic representation $\pi \mathfrak{W}(\mathcal{S})$ pertaining to $E \upharpoonright \mathcal{S}$ can be extended from $\mathfrak{W}(\mathcal{S})$ to $\mathfrak{W}(\mathcal{T})$ by specifying (within $\mathcal{B}(\mathcal{K})$)

$$\pi W(u) := \lim_{n \rightarrow \infty} \pi W(u_n) \quad , \quad \text{strongly in } \mathcal{B}(\mathcal{K}) \quad . \quad (**)$$

It follows

$$\begin{aligned} E(u) &= \lim_{n \rightarrow \infty} E(u_n) = \lim_{n \rightarrow \infty} \langle \Omega, \pi W(u_n) \Omega \rangle \\ &= \langle \Omega, \lim_{n \rightarrow \infty} \pi W(u_n) \Omega \rangle = \langle \Omega, \pi W(u) \Omega \rangle . \end{aligned}$$

So this extension is also cyclic for $\mathfrak{W}(\mathcal{T})$ with the same cyclic vector $\Omega \in \mathcal{K}$. Furthermore, due to (**), $\pi \mathfrak{W}(\mathcal{T})$ is in the strong closure of $\pi \mathfrak{W}(\mathcal{S})$ and hence even more so in the weak closure $[\pi \mathfrak{W}(\mathcal{S})]''$. □

For any representation π in $\mathcal{B}(\mathcal{H})$ according to STONE's theorem there are self-adjoint generators $R(u)$ in $\mathcal{H}$ of the unitary one-parameter groups $\pi W(tu)$ (note that $R(u) \notin \pi \mathfrak{W}(\mathcal{L}) \subset \mathcal{B}(\mathcal{H})$).

The *field algebra* of this representation is defined as the non-commutative free polynomial algebra over all monomials of the form

$$M = C R(u_1) \dots R(u_n) \quad (C \in \mathbb{C}, u_\nu \in \mathcal{L})$$

If the state ω is regular, i.e. $E = \omega \circ W$ is continuous on all rays of $\mathcal{L}$, then the GNS representation π of ω exists and we define the following expectation values

$$\omega(M) := C(i)^n \frac{\partial^n}{\partial t_1 \dots \partial t_n} \Big|_0 \omega(W(t_1 u_1) \dots W(t_n u_n)) \quad , \quad (2.2.1)$$

provided the corresponding derivatives exist. This definition is canonically extended over all elements of the field algebra.

In particular, the well-known *annihilator* and *generator* of a particle with wave function u are, respectively,

$$\begin{aligned} a(u) &= \frac{1}{\sqrt{2}} (R(u) + i R(u)) \\ a^*(u) &= \frac{1}{\sqrt{2}} (R(u) - i R(u)). \end{aligned}$$

The canonical commutation relations in the more traditional form (1.4) are then derived from (1.5), or equivalently from (WR), cf. page 11.

Finally, a state is said to be *gauge invariant*, if its generating functional satisfies

$$E(e^{it}u) = E(u) \quad ; \quad \text{for every } u \in \mathcal{L}, t \in \mathbb{R}$$

Examples Some generating functionals of regular states will be of particular interest to us. In the first place, these are the following so-called *Gauss functionals*.

Let $\mathcal{L}$ be a prehilbert space with closure $\overline{\mathcal{L}}$ and canonical symplectic form $\sigma(u, v) = \frac{1}{2} \Im \langle u, v \rangle$. Then

$$E_{\mathcal{F}}(u) := \exp\left(-\frac{1}{4} \|u\|^2\right)$$

is named the *Fock functional*. The most general Gauss functional is of the form:

$$E(u) = E_{\mathcal{F}} \exp\left(-\frac{1}{2} (u, u)\right), \quad (2.2.2)$$

with any sesquilinear positive form $(\cdot, \cdot)$ on $\mathcal{L}$.

If the form $(\cdot, \cdot)$ is even closeable on $\mathcal{D} \subset \overline{\mathcal{L}}$, then there exists exactly one positive self-adjoint operator A in $\overline{\mathcal{L}}$ with domain $\mathcal{D}$ such that $(u, u) = \|A(u)\|^2$, for all $u \in \mathcal{L}$ (see Appendix, p. 63 ff.) and with

$$T := (\mathbf{1} + A^2)^{\frac{1}{2}}$$

the functional (2.2.2) can also be written in the form

$$E(u) = \exp\left(\frac{1}{4} \|Tu\|^2\right).$$

So it is the Fock functional over $\mathcal{L}$ with the scalar product $\langle Tu, Tv \rangle$ instead of $\langle u, v \rangle$. Therefore states with generating Gauss functionals are also called *quasi-free*.

Quasi-free states are obviously gauge invariant and in their GNS representation expectation values exist for them for all polynomials of the field algebra in the In particular, one immediately verifies

$$\omega(a^*(u)a(v)) = (v, u). \quad (2.2.3)$$

The *reduction* of a Weyl*-system to any subsystem is straightforward in our formalism.

Let U, V be measurable in $\mathbb{R}^3$, $V \subset U$, and let $\mathcal{L}$ be a prehilbert space that is dense in $L^2(U)$ and such that $\mathcal{D}(V) \subset \mathcal{L}$ (for example $U = \mathbb{R}^3$ and $\mathcal{L} = L^2(\mathbb{R}^3)$).

Let moreover W be the Weyl*-system of $\mathfrak{W}(\mathcal{L})$. Then W_V , defined as

$$W_V := W \upharpoonright \mathcal{D}(V),$$

obviously is a Weyl*-system over $\mathcal{D}(V)$ and the subalgebra $\mathfrak{W}_V$ of $\mathfrak{W}(\mathcal{L})$ generated by W_V is *-isomorphic to the 'local' Weyl algebra over $\mathcal{D}(V)$. Physically, the latter represents a system in V as a subsystem of the system in U presented by $\mathfrak{W}(\mathcal{L})$.

Definition If ω is a state on $\mathfrak{W}(\mathcal{L})$, then the state obtained by restriction

$$\omega_V := \omega \upharpoonright \mathfrak{W}_V$$

is called the *local reduction* of ω to V .

If ω is even regular and the following sesquilinear form exists on $\mathcal{L}$

$$\omega(a^*(u)a(v)) \quad , \quad u, v \in \mathcal{L}$$

(which is $\mathbb{C}$ -linear in the first and anti $\mathbb{C}$ -linear in the second argument) and if moreover this form can be expressed with a Lebesgue measurable kernel $\mathcal{W}(x, y)$ as

$$\omega(a^*(u)a(v)) = \int_{U \times U} \mathcal{W}(x, y) u(x) \overline{v(y)} dx dy \quad , \quad (2.2.4)$$

then $\mathcal{W}$ is called the *two-point function* of ω , and ω_V obviously has the two-point function

$$\mathcal{W} \upharpoonright V \times V \quad .$$

It is also common to write $\langle a^*(x)a(y) \rangle$ instead of $\mathcal{W}(x, y)$.

Remark We still make the above assumptions, that is, U and V are measurable in $\mathbb{R}^3$, $V \subset U$, and $\mathcal{L}$ is a prehilber space in $\mathcal{H} = L^2(U)$ such that $\mathcal{D}(V) \subset \mathcal{L}$.

Then in the *Fock representation* of $\mathfrak{W}(\mathcal{L})$ (that is, the representation operating on the symmetric Fock space $\mathcal{F}(\mathcal{H})$), the reduction ρ_V of any state ρ represented by a density operator on $\mathcal{F}(\mathcal{H})$ is exactly the classical reduction of ρ known from quantum mechanics, i.e. the reduction of ρ by partial trace over the second factor in the tensor product

$$\mathcal{F}(\mathcal{H}) \cong \mathcal{F}(\mathcal{E}) \otimes \mathcal{F}(\mathcal{E}^\perp)$$

where $\mathcal{E} = L^2(V)$ and $\cong$ denotes the isomorphism of the Fock spaces induced by the direct sum decomposition

$$\mathcal{H} = \mathcal{E} \oplus \mathcal{E}^\perp$$

(cf. p. 44, Theorem 5.1.1 (1)).

Because under this isomorphism clearly holds for all $u \in \mathcal{D}(V)$ and $v \in \mathcal{E}^\perp$

$$w(u+v) \cong w(u) \otimes w(v) \quad ,$$

where each w stands for the corresponding Weyl system of the Fock representation, on which it operates, that is, on $\mathcal{F}(\mathcal{H})$, $\mathcal{F}(\mathcal{E})$, or $\mathcal{F}(\mathcal{E}^\perp)$, respectively.

In particular

$$w(u+0) \cong w(u) \otimes \mathbf{1} \quad ; \quad \text{for every } u \in \mathcal{D}(V) .$$

The above definition of the state ρ reduced to ρ_V then is equivalent (with the respective density operators likewise written ρ and ρ_v) to requiring equality of all expectation values

$$\begin{aligned} \text{Tr}[\rho_V w(u)] &= \text{Tr}[\rho(w(u) \otimes \mathbf{1})] \quad , \quad u \in \mathcal{D}(V) \\ &\quad (\text{Tr the trace}) , \end{aligned}$$

the solution ρ_V of which is the well-known reduced state known from quantum mechanics, cf. JAUCH [33], p. 179 ff.

Local reduction will be used especially to determine critical particle densities that produce Bose condensation in a thermodynamic volume limit. (cf. main theorems 5.1.2. and 5.3.1.).

2.3. Particles and Currents

We need to sharpen some more terms for our subsequent applications.

Let π be a Weyl system over a prehilbert space $\mathcal{L}$ with the representation space $\mathcal{H}$ and M be a finite-dimensional subspace of $\mathcal{L}$.

Definition We call the *counter of particles with wave function in M* the always existing unique self-adjoint operator $N(M)$ in $\mathcal{H}$ with the following properties

- (1) $0 \in \text{spec } N(M)$.
- (2) The unitary one-parameter group $e^{itN(M)}$ operates in the weak closure of $\pi \mathfrak{W}(M) \subset \pi \mathfrak{W}(\mathcal{L})$.
- (3) For every $u \in M$

$$e^{itN(M)} \pi W(u) e^{-itN(M)} = \pi W(e^{it}u) .$$

CHAIKEN [34], Proposition 3.1., shows that the spectrum of $N(M)$ consists of the natural numbers and that for every orthonormal Basis B of M

$$N(M) = \sum_{\mathbf{e} \in B} N([\mathbf{e}]) = \sum_{\mathbf{e} \in B} a^*(\mathbf{e}) a(\mathbf{e}) \quad ,$$

where $[\mathbf{e}]$ denotes the $\mathbb{C}$ -linear span of $\mathbf{e} \in B$.

In a regular state ω , the right-hand side of this equation yields via the expectation values for monomials of the field algebra, cf. page 13, a canonical definition of the expectation value

$$\omega(N(M))$$

for the number of particles with wave functions in M (π in this case being the GNS representation for ω).

In contrast to the counter of particles with wave function in a finite-dimensional subspace M of $\mathcal{L}$ (sometimes M is also referred to as the *space of 'modes'*), an operator of the total number of particles only exists under very special conditions for the representation π . The following theorem highlights an important class for the free Bose gas.

Theorem 2.3.1. (CHAIKEN, DELL'ANTONIO, DOPLICHER, RUELLE)

Let $\mathcal{L}$ be a separable prehilbert space, $T \geq \mathbf{1}$ an operator defined on the whole of $\mathcal{L}$, self-adjoint in the closure of $\mathcal{L}$, and ω a state on $\mathfrak{W}(\mathcal{L})$ with generating functional

$$E(u) = \exp\left(\frac{1}{4} \|Tu\|^2\right) .$$

Then the following statements are equivalent

- (1) The GNS representation π for ω is unitary equivalent to a direct sum of Fock representations, that is

$$\pi(A) = U \circ (\pi_{\mathcal{F}}(A) \otimes \mathbf{1}) \circ U^{-1} ; \quad A \in \mathfrak{W}(\mathcal{L}) ,$$

where U is a Hilbert space isomorphism, $\pi_{\mathcal{F}}$ is the Fock representation and $\mathbf{1}$ the identity in a certain Hilbert space $\mathcal{K}$.²

- (2) The operator

$$A := \frac{1}{\sqrt{2}} (T^2 - \mathbf{1})^{\frac{1}{2}}$$

is of the Hilbert-Schmidt type .

- (3) In the representation space $\mathcal{H}$ of π there exists exactly one self-adjoint operator N such that for all orthonormal bases $B = \{\mathbf{e}_n\}_{n \in \mathbb{N}}$ of $\mathcal{L}$

$$N = \sum_{\mathbf{e} \in B} N([\mathbf{e}])$$

in the sense of strong convergence for all elements in the domain of N .

Furthermore, if one of the statements (1), (2), (3) holds, then exists

$$\omega(N) := \text{Tr}_{\mathcal{L}} A^2 = \sum_{\mathbf{e} \in B} \omega(N([\mathbf{e}])) , \quad (2.3.1)$$

the spectrum of N are the natural numbers and

$$e^{itN} \pi W(u) e^{-itN} = \pi W(e^{it}u) , \quad \text{for all } u \in \mathcal{L} .$$

Proof: (1) $\iff$ (2) : CHAIKEN [35]
 (1) $\iff$ (3) : DELL'ANTONIO, DOPLICHER, RUELLE [36]

The last statement of the theorem with especially (2.3.1) is a trivial consequence of (2), (3) and equation (2.2.3),

² The equivalence to a direct sum of Fock representations then follows with $\mathcal{K}$ from the isomorphism $\mathcal{F} \otimes \mathcal{K} \cong \oplus_{\mathbf{e} \in B} \mathcal{F}$, with any basis B for $\mathcal{K}$.

with keeping in mind that

$$E(u) = E_{\mathcal{F}}(u) \exp\left(-\frac{1}{2}(u, u)\right) \quad \text{with} \quad (u, u) = \langle A^2 u, u \rangle.$$

The spectrum statement and the above connection with the gauge group $U(1)$ follow from (1) and corresponding statements for N in the Fock representation. $\square$

Definition If one of the above statements (1), (2) or (3) is true, then N is called the *particle number operator* and (2.3.1) is the expected value for the *total* number of particles in state ω .

For a class of states in which no particle number operator exists, local reduction to a volume with compact closure still leads to a state with a particle number operator. In this case we speak of *locally normal states*. Then particle densities and current densities can often be reasonably defined.

Let U be measurable in $\mathbb{R}^3$ and $\mathcal{D}(U) \subset \mathcal{L} \subset L^2(U)$. Let ω be a state on $\mathfrak{W}(\mathcal{L})$ with generating functional

$$E(u) = E_{\mathcal{F}}(u) \exp\left(-\frac{1}{2}(u, u)\right)$$

with a continuous kernel $\mathcal{W}(x, y)$, which is the two-point function of the sequilinear form

$$\omega(a^*(u)a(v)) = (v, u) = \int_{U \times U} \mathcal{W}(x, y) u(x) \overline{v(y)} dx dy$$

(cf. (2.2.3), (2.2.4)).

The requirements of Theorem 2.3.1 are then fulfilled for every local reduction ω_V of ω to a bounded open region $V \subset U$ with the integral operator A^2 defined by the kernel

$$\mathcal{W} \upharpoonright V \times V.$$

So there exists a particle number operator N for the state ω_V and according to (2.3.1)

$$\omega_V(N) = \text{Tr}_{\mathcal{D}(V)} A^2 = \int_V \mathcal{W}(x, x) dx.$$

Therefore, the following convention makes sense

Definition The diagonal of the two-point function of ω

$$\rho(x) := \mathcal{W}(x, x) =: \text{diag } \mathcal{W}(x, y) \quad (2.3.2)$$

is called the *particle number density* in the state ω .

Furthermore, we assign to the following triple $\mathbf{j}(u) = (j_\nu(u))_{\nu=1}^3$ of field algebra polynomials

$$j_\nu(u) := \frac{1}{2i} (a^*(\partial_\nu u) a(u) - a^*(u) a(\partial_\nu u)) \quad , \quad \nu = 1, 2, 3$$

the physical interpretation of the *particle stream with wave function* u .

If the two-point function of ω is continuously differentiable, then for every local reduction ω_V of ω to a bounded open region $V \subset U$ exists, independently of the choice of any orthonormal Basis $B = \{e_\mu\}_{\mu \in \mathbb{N}} \subset \mathcal{D}(V)$ for $L^2(V)$

$$\omega_V(\mathbf{j}) := \sum_{e \in B} \omega_V(\mathbf{j}(e))$$

and one verifies

$$\omega_V(\mathbf{j}) = \int_V \text{diag} \frac{i}{2} (\nabla_x - \nabla_y) \mathcal{W}(y, y) dx ,$$

where $\nabla \dots$ denotes the (complex) gradient in the indexed argument of $\mathcal{W}(x, y)$. It therefore makes sense to agree on the following usage of quantum field theory

Definition (1) The vector field on U

$$\mathbf{j}(x) := \text{diag} \frac{i}{2} (\nabla_x - \nabla_y) \mathcal{W}(x, y) \quad (2.3.3)$$

is called the (*particle*) *current density* in the state ω .

(2) This leads, again according to conventional quantum field theory, to defining

$$\epsilon(x) := \text{diag} \frac{1}{2} (\nabla_x \cdot \nabla_y) \mathcal{W}(x, y) \quad (2.3.4)$$

as the *density of the kinetic energy* in the state ω .

In (2) we use the notational convention

$$(\nabla_x \cdot \nabla_y) f(x, y) := \sum_{\nu=1}^3 \frac{\partial f}{\partial x_\nu} \frac{\partial f}{\partial y_\nu} ,$$

for any differentiable function $f : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{C}$.



3. Dynamics and Equilibrium

3.1. The Temporal Evolution

In quantum mechanics of systems with a finite number of degrees of freedom, the temporal evolution is generally represented by a weakly continuous one-parameter group of unitary transformations of a Hilbert space. Via STONE'S theorem, differential equations such as the Schrödinger or Heisenberg equations correspond to this description. In this case, the Hamilton operator simultaneously plays the role of the self-adjoint generator of the unitary one-parameter group and that of the operator of the (total) energy. In Bose systems with a finite number of degrees of freedom, VON NEUMANN'S representation theorem ensures the existence of essentially one irreducible representation of the canonical commutation relations. The description of symmetries of the system through unitary transformations in this representation as well as the temporal evolution through a one-parameter group of transformations arise here in a natural way.

In quantum field theory, an infinite number of degrees of freedom must be considered, which, as is well known, leads to the appearance of inequivalent representations of the canonical commutation relations. In order to exclude none of the potentially relevant ones from the outset, algebraic quantum field theory characterizes a dynamical system by a structure that is invariant under changes of representation, namely a universal C^* -algebra. The description of symmetries and dynamical evolutions of the system is then done canonically through isomorphisms of this structure, i.e. $*$ automorphisms of the underlying C^* -algebra.

Specifically, the temporal evolution is usually represented by a one-parameter group of $*$ automorphisms. In certain representations, this one-parameter group can be unitarily implemented, and it is not uncommon that an infinite number of self-adjoint generators of the dynamical one-parameter group exist in unitary inequivalent representations. As a rule, however, none of these self-adjoint operators may be identified with an observable of the system, especially no longer with the total energy in general.

In the following we will delve deeper into the dynamics of the interaction-free Bose gas, as prototypically observed in nature in helium 4. Due to the almost absence of internal interactions, the dynamics of the gas can be described by a Schrödinger equation in the test function (or "*wave function*") space.

Generally speaking, quasi-free Weyl systems such as those describing the infinite free Bose gas are characterized by the peculiarity that the dynamic automorphisms of $\mathfrak{W}(\mathcal{L})$ are induced by automorphisms of the symplectic space $\mathcal{L}$. Transformations of the C^* -algebra generated in this way are also called Bogoliubov transformations.

Definition (1) A *dynamical system* is any pair $(\mathcal{A}, \alpha)$ consisting of a C^* -algebra $\mathcal{A}$ and a one-parameter group

$$\alpha = \{\alpha_t\}_{t \in \mathbb{R}} \quad , \quad \alpha_{s+t} = \alpha_s \circ \alpha_t$$

of $*$ automorphisms of $\mathcal{A}$.

α is called the *dynamics* of the system $(\mathcal{A}, \alpha)$.

(2) A dynamics α that operates on the C^* -algebra $\mathfrak{W}(\mathcal{L})$ of a Weyl system is called *quasi-free* if it is induced by a one-parameter group $S = \{S_t\}_{t \in \mathbb{R}}$ of symplectic automorphisms of $\mathcal{L}$ satisfying

$$\alpha_t W(u) = W(S_t u) \quad , \quad t \in \mathbb{R}.$$

So in particular

$$S_{s+t} = S_s \circ S_t \quad \text{for every } s, t \in \mathbb{R}$$

and we shall speak simply of the *symplectic one-parameter group* S of $\mathcal{L}$.

(3) Specifically, we define the *infinite free Bose gas* as the dynamical system $(\mathfrak{W}(\mathcal{L}), \alpha)$ consisting of the tempered Weyl algebra over $\mathcal{L} = \mathcal{S}(\mathbb{R}^3)$ and the dynamics induced by the Laplace operator via

$$\alpha_t W(u) = W(e^{ith} u) ,$$

where h is the unique self-adjoint closure in $L^2(\mathbb{R}^3)$ of the operator on $\mathcal{S}(\mathbb{R}^3)$

$$-\frac{1}{2}\Delta - \mu \mathbf{1} \quad (\mu \in \mathbb{R}, \mu \leq 0).$$

μ is called the *chemical potential* of the Bose gas.

Convention If $(\mathcal{A}, \alpha)$ is a dynamical system and $A \in \mathcal{A}$, then we will often just write (αA) for the path

$$\begin{aligned} (\alpha A) : \mathbb{R} &\longrightarrow \mathcal{A} \\ t &\longmapsto \alpha_t(A) . \end{aligned}$$

3.2. The KMS Condition

If no energy operator exists, the classical description of the thermodynamic equilibrium using Gibbs canonical or grand canonical density operators is excluded. Due to the loss of extensive parameters, the distinction between different canonical ensembles already loses its meaning in the thermodynamic limit of infinite systems. The thermodynamic equilibrium of infinitely extended systems with an infinite number of degrees of freedom therefore needs to be recharacterized.

For this purpose, HAAG, HUGENHOLTZ and WINNING [21] proposed the use of the KUBO - MARTIN - SCHWINGER (KMS) boundary condition. In the case of finite

quantum systems, the condition characterizes precisely the Gibbs ensembles, but is equally suitable for characterizing the thermodynamic equilibrium of infinite systems. This is because it is formulated in terms of the general dynamics α above, i.e. independent of any special representations of the underlying C^* -algebra. The KMS condition circulates in several mathematically not entirely identical but physically essentially equivalent versions. A comparative overview is given by EMCH [28] (see also [29], [32]). In order to exclude any ambiguity from the outset, we commit ourselves to the version quoted below and already proposed by HAAG, HUGENHOLTZ and WINNINK [loc. cit. (3.31)]. Originally, the condition there takes the form of our KMS criterion below, cf. p. 23. The term '*simple*' boundary value we use refers to the convergence of a holomorphic function F in the sense of $\mathcal{S}'(\mathbb{R})$, i.e. the simple convergence in $\mathbb{C}^{\mathcal{S}(\mathbb{R})}$ (cf. KELLEY [37], p. 92.) Thereby we understand F as a functional on $\mathcal{S}(\mathbb{R})$ in the real part of the argument, with the imaginary part as a free parameter.

Definition Let $(\mathcal{A}, \alpha)$ be a dynamical system, $\beta \in \mathbb{R}_+$, and ω a state on $\mathcal{A}$. Then ω is called a *KMS state* with respect to the dynamics α and inverse temperature β if and only if the following applies:
For every $A, B \in \mathcal{A}$ there exists a tempered³ holomorphic function F on the strip $0 < \text{Im}(z) < \beta$ with continuous simple boundary value satisfying

$$\begin{array}{ll} \omega(B(\alpha_t A)) & \text{on the real axis} \\ \text{and} & \\ \omega((\alpha_t A)B) & \text{on the upper boundary } \mathbb{R} + i\beta \\ & \text{of the strip.} \end{array}$$

HAAG, HUGENHOLTZ and WINNINK [21] were the first to point out the KMS property as strictly characterizing Gibbs states in the finite volume and their limit states in the limit of infinitely extended systems. In 1974, HAAG, KASTLER and TRYCH-POHLMAYER [22] recognized the KMS condition as essentially equivalent to the stability of pure stationary phases against local perturbations of the dynamics and PUSZ and WORONOWICZ [36] recently discussed the direct connection between the KMS condition and the Second Law of Thermodynamics (passivity of the KMS states).

In contrast to the uniquely determined classical grand canonical ensemble of a finite system, in an infinite dynamical system there generally exist different KMS states of the same temperature. From the above definition it is immediately clear that the KMS states of the same temperature form a convex set. Two different states can therefore be transformed into each other completely within the set and continuously in the weak*-topology of states by varying a single parameter. Physically, this is interpreted as the presence of phase transitions between different equilibrium states of the system. Theorems 3.2.2 and 3.2.3 below describe relations between different KMS states on the Weyl algebra and allow to construct a large number of new KMS states for the same quasi-free dynamics and inverse temperature β from any given ones. In the proof of the theorems we apply the following useful *KMS criterion*. As usual, $\mathcal{Z}$ will denote the space of all Fourier transforms of complex valued C^∞ -functions with compact support in $\mathbb{R}$. The functions in $\mathcal{Z}$ are canonically holomorphic and even entire on all of $\mathbb{C}$, see e.g. [39], Chapter II.

³ i.e. not increasing faster than a polynomial

KMS criterion The KMS condition for ω is equivalent to the following property:
For all $A, B \in \mathcal{A}$ and $\phi \in \mathcal{Z}$ holds

$$\int_{\mathbb{R}} \phi(t) \omega((\alpha_t A) B) dt = \int_{\mathbb{R}} \phi(t - i\beta) \omega(B(\alpha_t A)) dt. \quad (*)$$

Proof: For simplicity, we write Fourier transformation shortly as $\widehat{\phi}$, where the argument of ϕ (t or p) always determines which one is meant. So, with

$$\mathfrak{F}(\phi(t)) := \int_{\mathbb{R}} e^{-ipt} \phi(t) dt \in \mathcal{Z}, \quad \phi(t) \in \mathcal{D}(\mathbb{R}),$$

$\widehat{\phi}(p) := \mathfrak{F}(\phi(t)) \in \mathcal{Z}$, for $\phi(t) \in \mathcal{D}(\mathbb{R})$ and $\widehat{\phi}(t) := \mathfrak{F}^{-1}(\phi(p)) \in \mathcal{D}(\mathbb{R})$, for $\phi(p) \in \mathcal{Z}$. The argument always makes clear which Fourier transform is meant.

Note that by replacing $p \in \mathbb{R}$ with $z \in \mathbb{C}$ in $\widehat{\phi}(p) = \int_{\mathbb{R}} e^{-ipt} \phi(t) dt$, this function is holomorphically continued to all of $\mathbb{C}$.

Relation $(*)$ is equivalent to

$$e^{\beta p} \widehat{f}(p) = \widehat{g}(p) \quad \text{in } \mathcal{S}'(\mathbb{R}), \quad (4)$$

where $f(t) = \omega((\alpha_t A) B)$ and $g(t) = \omega(B(\alpha_t A))$. This yields the KMS condition in the form of the initial definition from general theorems about boundary values of analytic functions, see for example BELTRAMI and WOHLERS [39], theorems 2.1 and 2.4. [In order to derive there the $\mathcal{S}'(\mathbb{R})$ boundary value property for the function $F(z)$ from the $\mathcal{Z}'$ boundary value property (Theorem 2.4), one shows that

$$e^{sp} \widehat{f}(p) \quad \text{is continuous in } \mathcal{S}'(\mathbb{R}) \text{ with respect to } s \in [0, \beta]. \quad (**)$$

This follows this way: As a functional of $\mathcal{S}'(\mathbb{R})$, $\widehat{f}(p)$ can be written in the form

$$D^l((1 + p^2)^{m/2} h(p)),$$

with $l, m \in \mathbb{N}$ and a bounded continuous function $h(p)$ on the real line. see L. SCHWARTZ [40], Theorem IV, p. 239 (also cited in BELTRAMI and WOHLERS [39], Theorem 1.28, p. 36). (The derivative D^l of course denotes the weak derivative in $\mathcal{S}'(\mathbb{R})$, i.e. in the distributional sense.) Applying the functional $(**)$ to $\phi \in \mathcal{S}(\mathbb{R})$ then yields

$$e^{sp} \widehat{f}(p) [\phi(p)] = \int_{\mathbb{R}} (-1)^l D^l(e^{sp} \phi(p)) (1 + p^2)^{m/2} h(p) dp.$$

Now the $\mathcal{S}'(\mathbb{R})$ -continuity with respect to $s \in [0, \beta]$ of $e^{sp} \widehat{f}(p)$ follows from the theorem about the continuous dependence of an integral on a continuous parameter in the integrand.]

Conversely, the condition $(*)$ follows from the initial definition of KMS states via an $\epsilon/2$ argument for

$$\int_{\mathbb{R}} \phi(t - is) F(t + i(\beta - s)) dt \quad (\phi \in \mathcal{Z})$$

using Cauchy's integral theorem. [When shifting the integral from $s = 0$ to $s = \beta$, note that the function $\phi(t - is) F(t + i(\beta - s))$ for $s \in (0, \beta)$ disappears uniformly at infinity, since F is tempered.] □

⁴ With BOCHNER's theorem, this results in particular in the well-known time translation invariance of KMS states by simply setting $B := \mathbf{1}_{\mathcal{A}}$.

Lemma 3.2.1. Let ω be a KMS state on the Weyl algebra $\mathfrak{W}(\mathcal{L})$ for any dynamics α and inverse temperature β , and let $\tilde{\omega}$ be a stationary state on $\mathfrak{W}(\mathcal{L})$, such that a bounded symmetric $\mathbb{C}$ -valued functional m exists on $\mathcal{L} \times \mathcal{L}$ which for all $u, v \in \mathcal{L}$ on the whole of $\mathbb{R}$ satisfies

$$\tilde{\omega}(W(u)(\alpha_t W(v))) = m(u, v) \omega(W(u)(\alpha_t W(v))) . \quad (*)$$

Then also $\tilde{\omega}$ is KMS with respect to α and β .

Proof: From $(*)$ and the KMS property of ω it first follows that for every $\phi \in \mathcal{Z}$ and $u, v \in \mathcal{L}$

$$\int_{\mathbb{R}} \phi(t) \tilde{\omega}((\alpha_t W(u))W(v)) dt = \int_{\mathbb{R}} \phi(t-i\beta) \omega(W(v)W(\alpha_t W(u))) dt . \quad (**)$$

Due to the Weyl relations (WR), see p. 11, this immediately extends to all elements of every algebra finitely generated from Weyl elements $W(u)$, $u \in \mathcal{L}$. Since $\tilde{\omega}((\alpha_t X)Y)$ is a bounded function of t and is continuous in $X, Y \in \mathfrak{W}(\mathcal{L})$ for every fixed t , $(**)$ holds even for every $A, B \in \mathfrak{W}(\mathcal{L})$ in the place of $W(u), W(v)$, due to Lebesgue's bounded convergence theorem.

This is shown using A and B approximating series of linear combinations of Weyl elements. Applying the Weyl relations (WR) and given the boundedness of ω on the unit sphere of $\mathfrak{W}(\mathcal{L})$, one obtains due to the continuity of $\omega((\alpha_t X)Y)$ and $\omega(Y(\alpha_t X))$ on $\mathbb{R}$ and the boundedness of the functional m , uniformly convergent sequences of bounded continuous functions on $\mathbb{R}$, which converge to the then also continuous functions $\omega((\alpha A_t)B)$ and $\omega(B(\alpha_t A))$, respectively. □

Direct consequences of the above lemma are the following two theorems about KMS states of a quasi-free dynamics on the Weyl algebra.

Theorem 3.2.2. Let α be a quasi-free dynamic on $\mathfrak{W}(\mathcal{L})$ with symplectic one-parameter group $S = \{S_t\}_{t \in \mathbb{R}}$ acting on $\mathcal{L}$, and let ω be a state on $\mathfrak{W}(\mathcal{L})$ with generating functional $E = \omega \circ W$ and such that ω is extremal KMS with respect to α and β . Furthermore, let $F : \mathcal{L} \rightarrow \mathbb{R}$ be a real-linear function on $\mathcal{L}$ that is invariant with respect to S (i.e. $F = F \circ S$). Then every state $\tilde{\omega}$ with generating functional

$$\tilde{E}(u) = e^{iF(u)} E(u) , \quad u \in \mathcal{L} \quad (\dagger)$$

is also an extremal KMS state for α and β .

Proof: With Lemma 3.2.1. it is immediately verified that $\tilde{\omega}$ is a KMS state, since $(*)$ is obviously satisfied with

$$m(u, v) := e^{iF(u+v)} , \quad \text{for all } u, v \in \mathcal{L} .$$

Furthermore, if $\tilde{\omega}$ were not extremal but a mixture of at least two different KMS states $\tilde{\omega}_1, \tilde{\omega}_2$ (which themselves may be extremal or mixtures),

that is, $\tilde{\omega}$ can be written with any $t \in (0, 1)$ as

$$\tilde{\omega} = s\tilde{\omega}_1 + (1-s)\tilde{\omega}_2 ,$$

then because of $(\dagger)$, conversely

$$E = s e^{-iF} \tilde{E}_1 + (1-s) e^{-iF} \tilde{E}_2 ,$$

so that ω would also be a mixture, contrary to the assumption. $\square$

The next theorem also follows directly from Lemma 3.2.1. Let $\mathcal{R}$ denote an arbitrary sigma ring of real-valued, real-linear functionals on $\mathcal{L}$, invariant under the operation of the symplectic one-parameter group $S = \{S_t\}_{t \in \mathbb{R}}$ on $\mathcal{L}$. And let ω be a KMS state on $\mathfrak{W}(\mathcal{L})$ for inverse temperature β and quasi-free dynamics α induced by S , with generating functional $E = \omega \circ W$. Then the following holds.

Theorem 3.2.3. (ROCCA, SIRUGUE, TESTARD)

If μ is any measure on $\mathcal{R}$ of total mass 1 and such that all mappings

$$\begin{aligned} (u) : \mathcal{R} &\longrightarrow \mathbb{R} \quad , \quad u \in \mathcal{L} \\ F &\longmapsto F(u) \end{aligned}$$

are μ measurable, then the functional

$$\tilde{E}(u) = \int_{\mathcal{R}} e^{iF(u)} E(u) d\mu(F) \quad , \quad u \in \mathcal{L}$$

is the generating functional of a KMS state $\tilde{\omega}$ for α and β .

Proof: Trivial consequence of lemma 3.2.1 with

$$m(u, v) := \int_{\mathcal{R}} e^{iF(u+v)} d\mu(F) \quad , \quad \text{for all } u, v \in \mathcal{L} .$$

$\square$

Corollary (Main application example)

For any $n \in \mathbb{N}_+$ let $\mathcal{R}$ be the n -dimensional real vector space spanned by n linearly independent real-valued $\mathbb{R}$ -linear S -invariant functionals $F_1, \dots, F_n$ on $\mathcal{L}$, and let $x_1, \dots, x_n$ be the dual basis of $F_1, \dots, F_n$. Then the quadratic form $x_1^2 + \dots + x_n^2$ makes $\mathcal{R}$ a Euclidean vector space isomorphic to $\mathbb{R}^n$ and a Borel-measure space $(\mathcal{R}, d\mu(F))$ via the Gaussian normal distribution imported from $\mathbb{R}^n$. With Theorem 3.2.3 then holds

$$\begin{aligned} \tilde{E}(u) &= \int_{\mathcal{R}} e^{iF(u)} E(u) d\mu(F) \\ &= E(u) (2\pi)^{-\frac{n}{2}} \prod_{\nu=1}^n \int_{\mathbb{R}} e^{i x_{\nu} F_{\nu}(u) - \frac{x_{\nu}^2}{2}} dx_{\nu} \end{aligned}$$

that is

$$\tilde{E}(u) = E(u) \exp\left(-\frac{1}{2} \sum_{\nu=1}^n F_{\nu}(u)^2\right) .$$

Note that there is a connection between Theorem 3.2.3. and the central decomposition theorem. Under additional conditions for the quasi-free dynamics (so far we have not yet imposed any further restrictions on it), ROCCA, SIRUGUE and TESTARD [9] indeed obtain a tightened form of Theorem 3.2.3. According to this, every (in the sense of (2.2.1), p. 13) C^∞ -differentiable KMS state of such a dynamic allows an integral representation in the form given in Theorem 3.2.3. with the generating functional E of a suitable extremal time invariant state. This integral representation then turns out to be the central decomposition (loc. cit., Theorem 4.10).

3.3. The Role of the Laplace Equation

The theorems of the previous section point to the importance of S_t -invariant functionals on a general symplectic space $\mathcal{L}$ of the Weyl algebra $\mathfrak{W}(\mathcal{L})$ for the description of the thermodynamic equilibrium of a quasi-free dynamic. In this section we classify the continuous real-linear functionals on $\mathcal{L} = \mathcal{S}(\mathbb{R}^3)$ which are invariant under the one-particle dynamics $S_t = e^{ith}$ of the free Bose gas (see page 21, Definition (3)). The Laplace equation appears here as a time-independent Schrödinger equation. However, in contrast to the lowest one-particle eigenstates of a Schrödinger equation, we are interested in solutions of the Laplace equation a more general distributional sense. This has certain consequences for the interpretation of the long-range order parameter of the Bose condensate.

In the following let $\mathfrak{W}$ denote the tempered Weyl algebra over $\mathcal{L} = \mathcal{S}(\mathbb{R}^3)$ and α the free dynamics in $\mathfrak{W}$ given by:

$$\alpha_t W(u) = W(e^{ith} u) \quad , \quad u \in \mathcal{S}(\mathbb{R}^3)$$

with the self-adjoint operator h in $L^2(\mathbb{R}^3)$, which is the unique closure of

$$-\frac{1}{2} \Delta - \mu \quad , \quad \mu \leq 0 \quad \text{the chemical potential} \quad .$$

Furthermore, let for the so-called fugacity $\zeta := e^{\beta\mu}$ the function $w_\zeta : \mathbb{R}^3 \rightarrow \mathbb{R}$ be defined as

$$w_\zeta := (2\pi\beta)^{-\frac{3}{2}} \sum_{n=1}^{\infty} n^{-\frac{3}{2}} \zeta^n \exp\left(-\frac{x^2}{2n\beta}\right)$$

and let $*$ denote the convolution in $\mathbb{R}^3$. Then it is known that

$$E_\zeta(u) = E_{\mathcal{F}}(u) \exp\left(-\frac{1}{2} \langle w_\zeta * u, u \rangle\right) \quad (3.3.1)$$

is the generating functional of an extremal KMS state ω with respect to α and β which obviously is invariant under Euclidean transformations of $\mathbb{R}^3$. The extremal KMS property of ω is proven, for example, in DUBIN [41], p. 67 ff.

From Theorems 3.2.2 and 3.2.3. above, the importance of the following propositions in Lemma 3.3.1. for the description of the thermodynamic equilibrium of the free Bose gas becomes immediately clear.

Lemma 3.3.1. The *continuous* real-valued and real-linear functionals on $\mathcal{S}(\mathbb{R}^3)$ which are invariant with respect to e^{ith} are

- (1) in the case $\mu < 0$, only the zero distribution ⁽⁵⁾,
- (2) in the case $\mu = 0$, all distributions of the form

$$F(u) = \operatorname{Re}(Q[u]) \quad ,$$

with a solution polynomial Q of the Laplace equation, where $Q[u]$ denotes the application of Q to $u \in \mathcal{S}(\mathbb{R}^3)$ as the tempered distribution, i.e.

$$Q[u] = \int_{\mathbb{R}^3} \overline{Q(x)} u(x) dx \quad .$$

Proof: It is sufficient to show that the family of equations for $X \in \mathcal{S}'(\mathbb{R}^3)$

$$X \circ (e^{ith} - 1) = 0 \quad \text{for all } t \in \mathbb{R} \quad , \quad (A)$$

for $\mu < 0$ only admits the single solution $X = 0$ and for $\mu = 0$ it is satisfied by all solution polynomials Q of the Laplace equation ⁶.

Because for every solution X of equation (A) the functional $F := \operatorname{Re}(X[u])$ is clearly invariant with respect to e^{ith} , continuous, real-valued and real-linear. And conversely, for every such F , the $\mathbb{C}$ -valued functional $X[u] := F(u) - iF(iu)$ is a solution of (A) with $F(u) = \operatorname{Re}(X[u])$. So if only the solution polynomials of Laplace's equations satisfy equation (A), all distributions of the required type are covered.

After Fourier transformation (A) becomes

$$\begin{aligned} \widehat{X}[v] &= 0 \\ v(p) &= (e^{it((p^2/2)-\mu)} - 1) u(p) \end{aligned} \quad (B)$$

for every $u \in \mathcal{R}(\mathbb{R}^3)$ and $t \in \mathbb{R}$.

For $\mu < 0$ and any $p_0 \in \mathbb{R}^3$, there is obviously always a $t_0 \in \mathbb{R}$ such that

$$f(t, p) := e^{it(\frac{p^2}{2}-\mu)} - 1$$

does not disappear in t_0 . So p_0 does not belong to the support of any solution $\widehat{X}$ of (B). Since p_0 was arbitrary, $\widehat{X}$ has empty support and is therefore the zero distribution.

For $\mu = 0$, $p = 0$ is the only point in $\mathbb{R}^3$ at which $f(t, p)$ vanishes for all $t \in \mathbb{R}$. Therefore, every solution of (B) is concentrated in $0 \in \mathbb{R}^3$ and is therefore a linear combination of finitely many derivatives of the delta functional $\delta(p)$ (cf. GELFAND and SHILOV [42], vol. 1, p. 146).

⁵ Note, however, that for a dense subspace of *analytical* test functions $\mathcal{T}(\mathbb{R}^3) \subset \mathcal{S}(\mathbb{R}^3)$ singular e^{ith} invariant functionals exist for *every* chemical potential $\mu < 0$; cf. [55].

⁶ These polynomials are also called *Maxwell polynomials* and if they are homogeneous, *harmonic polynomials*.

$\widehat{X}$ can therefor be written, with a certain $m \in \mathbb{N}$ and suitable constants c_{τ} , $\tau \in \mathbb{N}^3$, in the form

$$\widehat{X}(p) = \sum_{|\tau| \leq m} c_{\tau} D^{\tau} \delta(p), \quad (C)$$

where

$$|\tau| := \tau_1 + \tau_2 + \tau_3 \quad \text{and} \quad D^{\tau} := \frac{\partial^{|\tau|}}{\partial p_1^{\tau_1} \partial p_2^{\tau_2} \partial p_3^{\tau_3}}$$

Now show by complete induction:

$$\frac{\partial^{2n}}{\partial p_j^{2n}} f = e^{it \frac{p^2}{2}} \sum_{\nu=0}^n (it)^{n+\nu} \frac{(2n)! p_j^{2\nu}}{2^{n-\nu} (n-\nu)! (2\nu)!} \quad (n > 0)$$

and

$$\frac{\partial^{2n+1}}{\partial p_j^{2n+1}} f = e^{it \frac{p^2}{2}} \sum_{\nu=0}^n (it)^{n+\nu} \frac{(2n+\nu)! p_j^{2\nu+1}}{2^{n-\nu} (n-\nu)! (2\nu+1)!} \quad (n \geq 0).$$

From this it follows

$$D^{\tau} f(t, 0) = \begin{cases} 0 & \text{if } \tau = 0 \text{ or at least one index } \tau_j \text{ is odd} \\ (it)^{\frac{|\tau|}{2}} \prod_{j=1}^3 \frac{\tau_j!}{(\tau_j/2)!} & \text{if all } \tau_j \text{ are even ('}\tau \text{ even')} \text{ and } |\tau| > 0. \end{cases}$$

Therefore

$$\begin{aligned} \widehat{X}[(e^{it \frac{p^2}{2}} - 1) u(p)] &= \int_{\mathbb{R}^3} \delta(p) \sum_{|\tau| \leq m} (-1)^{|\tau|} c_{\tau} D^{\tau} (fu) dp = \\ &= \sum_{\substack{\tau, \sigma \\ |\tau| \leq m \\ \sigma \text{ even} \\ 2 \leq |\sigma| \leq m - |\tau|}} (-1)^{|\tau|} (-it)^{|\sigma|/2} c_{\tau+\sigma} \left(\prod_{j=1}^3 \frac{(\tau_j + \sigma_j)!}{\tau_j! (\sigma_j/2)!} \right) (D^{\tau} u)(0). \end{aligned}$$

In this we applied the Leibniz rule for $D^{\tau}(fu)$, integrated and substituted the above expression for $D^{\tau}f(t, 0)$.

In order for the last expression to disappear for each $u \in \mathcal{S}(\mathbb{R}^3)$, the following must hold

$$\sum_{\substack{\sigma \text{ even} \\ |\sigma|=n}} c_{\tau+\sigma} \prod_{j=1}^3 \frac{(\tau_j + \sigma_j)!}{\tau_j! (\sigma_j/2)!} = 0, \quad (D)$$

for all positive even $n \leq m - |\tau|$.

The Fourier transform of (C) in $\mathcal{S}'(\mathbb{R}^3)$ is

$$X(x) = \sum_{|\tau| \leq m} (i)^{|\tau|} c_{\tau} x^{\tau}$$

wherein is set $x^{\tau} := x_1^{\tau_1} x_2^{\tau_2} x_3^{\tau_3}$.

From The Laplace equation $\Delta X = 0$ one calculate2 in the elementary way that the coefficients c_{τ} of X must satisfy the following condition for all $|\tau| \leq m - 2$

$$\sum_{\substack{\sigma \text{ even} \\ |\sigma|=2}} c_{\tau+\sigma} \prod_{j=1}^3 \frac{(\tau_j + \sigma_j)!}{\tau_j! (\sigma_j/2)!} = 0 , \quad (\text{E})$$

which is the special case of (D) with $n = 2$.

The reverse implication (E) $\implies$ (D) follows with some combinatorics. $\square$

As an immediate consequence of the lemma and the theorems of the previous section one obtains the following

Theorem 3.3.2. Let $\mu = 0$.

For every solution polynomial Q of the Laplace equation in $\mathbb{R}^3$ (which are all canonically distributions in $\mathcal{S}'(\mathbb{R}^3)$) these two statements apply

$$(1) \quad \tilde{E}(u) = e^{i\sqrt{2} \operatorname{Re}(Q[u])} E_1(u) , \quad u \in \mathcal{S}(\mathbb{R}^3) \quad (3.3.2)$$

is the generating functional of an *extremal* (generally not gauge invariant) KMS state $\tilde{\omega}$ on $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ for the dynamics α and inverse temperature β . (The definition of E_1 see (3.3.1) on p. 26).

$$(2) \quad \tilde{E}(u) = e^{-\frac{1}{2} |Q[u]|^2} E_1(u) , \quad u \in \mathcal{S}(\mathbb{R}^3) \quad (3.3.3)$$

is the generating functional of a quasi free, in particular *gauge invariant* KMS state $\tilde{\omega}$ on $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ for α and β .

Proof: (1): lemma 3.3.1. and Theorem 3.2.2.

(2): lemma 3.3.1. and Theorem 3.2.3.; application example with

$$\begin{aligned} F_1 &:= \operatorname{Re}(Q[\cdot]) \\ F_2 &:= \operatorname{Re}(iQ[\cdot]) = -\operatorname{Im}(Q[\cdot]) . \end{aligned}$$

$\square$

Remark The factors $\sqrt{2}$ in the exponent of (3.3.2) and $\frac{1}{2}$ in the exponent of (3.3.3), which are completely irrelevant to the statements of the theorem, only fulfill a normalization function with regard to (4.1.1).

Symbolically, we can represent the connection between (A) on page 27 and the Laplace equation in loose form like this

$$\frac{\partial}{\partial t} \Big|_{t=0} X \circ (e^{ith} - 1) = X \circ \frac{\partial}{\partial t} \Big|_{t=0} (e^{ith} - 1) = i X \circ h = 0 ,$$

where $h = -\frac{1}{2} \Delta$.

The equation

$$X \circ h = X \circ \left(-\frac{1}{2} \Delta\right) = 0$$

is the Laplace equation in the space of tempered distributions (i.e. with $X \in \mathcal{S}'(\mathbb{R}^3)$) and represents the differential version of equation (A). In fact, we are interested in the Maxwell polynomials Q as *weak solutions* of the Laplace equation, as suggested by Theorems 3.2.2. and 3.2.3. and as becomes clear in the proof of Lemma 3.3.1.

In Section 4 they will gain concrete importance as the classical fields that determine the typical particle correlations in the free Bose gas and especially the hydrodynamics of the Bose condensate.

A next natural step in clarifying the influence of any interactions between the particles on the diverse manifestations of the Bose condensate would be the introduction of an interaction potential in the one-particle Hamiltonian h . For this purpose, for example, a term $M(x)$ can be introduced into the Hamiltonian h which describes the interaction in a mean field approximation. The (still quasi-free) dynamics α on $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ would then be induced by

$$h = -\frac{1}{2} \Delta + M(x) - \mu . \quad (3.3.4)$$

[The term $M(x) - \mu$ is sometimes referred to as a "local" chemical potential.] The traditional formalism of field theory shows us the direction of further proceeding. The fictitious Hamiltonian of a system with a pair interaction is usually written as

$$H = \frac{1}{2} \int_{\mathbb{R}^3} |\vec{\nabla} a^*(x)|^2 dx + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \Phi(x-y) a^*(x) a^*(y) a(x) a(y) dx dy , \quad (3.3.5)$$

where Φ represents any interaction potential. The approximation now consists of replacing in H

$$a^*(x) a^*(y) a(x) a(y) \quad \text{with} \quad a^*(x) a(x) < a^*(y) a(y) > , \quad (3.3.6)$$

the expected value $< \dots >$ referring to an anticipated state in which the system will approximately be in equilibrium. The commutation of the operators (3.3.6) carried out in (3.3.5) provides an additional constant shift in the energy of each particle, which can, however, be attributed to the chemical potential μ . For the average potential acting on each individual particle we then get from (3.3.5) with (3.3.6)

$$M(x) = \int_{\mathbb{R}^3} \Phi(x-y) < a^*(y) a(y) > dy . \quad (3.3.7)$$

In the simplest case, if we describe the interaction by a Dirac measure

$$\Phi(x-y) = \lambda \delta(x-y) ,$$

then the average potential becomes according to (3.3.7)

$$M(x) = \lambda \langle a^*(x) a(x) \rangle .$$

In anticipation of the results of the next section, according to which the equilibrium states of the free Bose gas at low temperatures approximately satisfy

$$\langle a^*(x) a(x) \rangle = |Q(x)|^2 .$$

With 3.3.4 we get the following analogue of the Laplace equation

$$-\frac{1}{2} \Delta X + \lambda |X|^2 X - \mu X = 0 ,$$

which is the Ginzburg-Landau equation with the elementary charge set to zero.

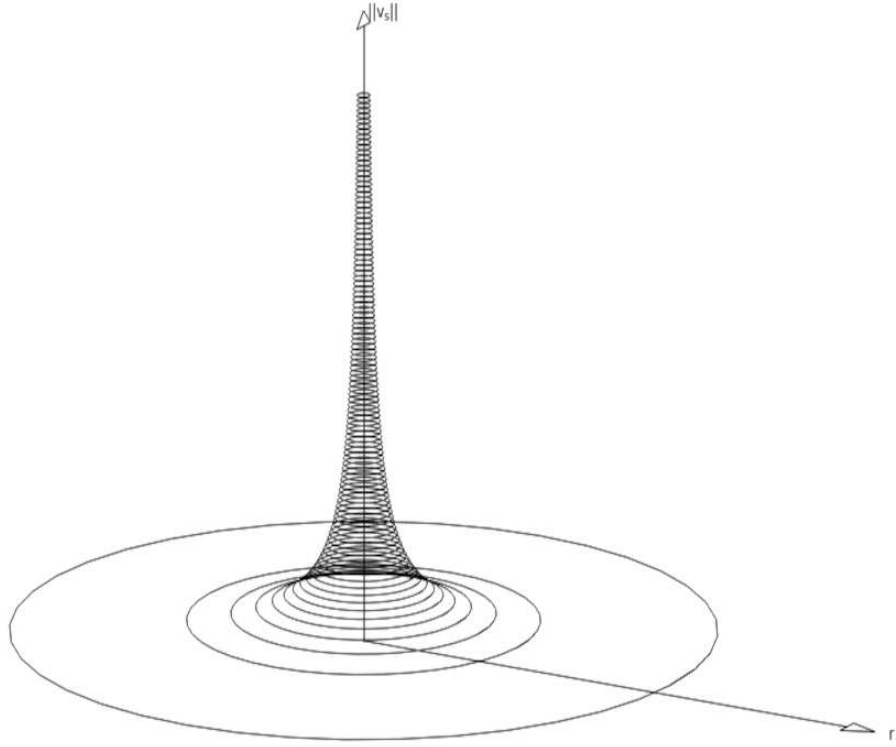


Fig. 2. The graph $\|v_s(r)\|$ of a simple vortex in the flow $v_s = \mathcal{I}m(Q^{-1}\nabla Q)$ with Q from (4.3.6), p. 38. $\|v_s(r)\|$ becomes singular of order $1/r$ for $r \rightarrow 0$.

4. The Hydrodynamic Picture

4.1. Typical Two-Point Correlations

Physically, the extremal KMS states of the form (3.3.2) represent the *pure phases* of the free Bose gas with chemical potential $\mu = 0$ in thermodynamic equilibrium. We call their two-point correlations *typical*. Every state ω on the tempered Weyl algebra $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ with generating functional (3.3.2) is regular, see p. 13, and even differentiable in every order in the sense of (2.2.1). Therefore, all expectation values of the field algebra exist for ω (see p. 13). Especially, using (2.2.1), we immediately calculate the two-point correlations or so-called *two-point function* of ω as

$$\mathcal{W}(x, y) = \overline{Q(x)} Q(y) + w_1(x - y) . \quad (4.1.1)$$

As is easily verified, the quasi-free (hence gauge invariant) state with generating functional (3.3.3) has the same two-point function (4.1.1). In particular, for every typical two-point correlation, there exists a gauge-invariant KMS state with the same correlation. Apparently this state is generally not extremal KMS, which however plays no role in its hydrodynamics. This will be seen in the following sections. So far, only states of the free Bose gas with a constant two-point correlation $\overline{Q}Q = \text{const}$ in the condensate have been investigated together with their physical properties. Like these, all states with symmetry-breaking two-point correlations of the type (4.1.1.) exhibit off-diagonal long-range order.

The typical two-point correlations suggest a natural two-component interpretation of these equilibrium states. The connection to the usual two-fluid model is made clear by the following convention

Definition For any state ω with two-point correlation (4.1.1), we call

$$\rho_s(x) := \overline{Q(x)} Q(x) \quad (4.1.2)$$

the *density of the superfluid phase*, and

$$\rho_n(x) := w_1(0) = (2\pi\beta)^{-\frac{3}{2}} \zeta\left(\frac{3}{2}\right) = (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(1) \quad (7) \quad (4.1.3)$$

the *density of the normal phase* in the state ω .

While the translation- and rotation-invariant two-point function $w_1(x - y)$ of the normal component decreases exponentially with $|x - y| \rightarrow \infty$, the correlation function $\overline{Q(x)}Q(y)$ associated with the superfluid phase shows long-range order and, in general, a breaking of Euclidean symmetry. So with good reason we can identify (4.1.2) as the density of the Bose condensate.

⁷ $\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$ is the *Riemann zeta function* (not to be confused with the fugacity $\zeta = e^{\beta\mu}$), and $g_z(s) = \sum_{n=1}^{\infty} \frac{s^n}{n^z}$ the commonly used generalization of the zeta function.

Of course, Theorem 3.2.3. also leads to KMS states with other two-point correlations, for example

$$\mathcal{W}(x, y) = \sum_{\nu=0}^n \overline{Q_\nu(x)} Q_\nu(y) + w_1(x - y). \quad (4.1.4)$$

For all *extremal* KMS states of the form $(\dagger)$ in Theorem 3.2.2. with a continuous functional F (and setting $E = E_1$), according to the results of Section 3.3. only particle correlations of the form (4.1.1) can occur. We therefore consider and call the two-point functions (4.1.4) *atypical*. As *mixtures* of extremal KMS states they correspond to a lower level of knowledge about the state of the system, and are easily generated following the pattern of Theorem 3.2.3.

[This is easily seen by setting in the Main application example on p. 25 $E := E_1$, see (3.3.1) with $\zeta = 1$, and for $\nu = 1, \dots, n$

$$\begin{aligned} F_{2\nu-1}(u) &:= \operatorname{Im}(Q_\nu[u]) \\ F_{2\nu}(u) &:= \operatorname{Re}(Q_\nu[u]) \quad , \quad \text{for every } u \in \mathcal{S}(\mathbb{R}^3) \end{aligned}$$

Essentially due to Lemma 3.3.1, no Bose condensate occurs for $\mu < 0$. In this case, the state associated to E_z with the two-point function

$$w_z(x - y)$$

represents the only equilibrium phase of the Bose gas.

The two-component interpretation laid down in the previous definition for the case $\mu = 0$ seems natural in view of (4.1.1). This interpretation leads to a canonical hydrodynamics of the free Bose condensate developed in the following section. Some of its characteristic properties can easily be generalized to a larger class of states, since they result directly from the general form $\overline{q(x)}q(y)$ of the particle correlation in the condensate.

4.2. Quantized Vortices

Regardless of the equilibrium situation or even a special dynamics for $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$, we first study properties of states that allow a canonical two-component interpretation, as in example (4.1.1). This is then applied to the free Bose gas.

Let $\mathfrak{W}(\mathcal{L})$ be a Weyl algebra over a prehilbert space $\mathcal{L}$ that is dense in $L^2(\mathbb{R}^3)$ and ω a state $\mathfrak{W}(\mathcal{L})$ with a continuously differentiable two-point function

$$\mathcal{W}(x, y) = \overline{q_\nu(x)}q_\nu(y) + w(x - y). \quad (4.2.1)$$

where $q : \mathbb{R}^3 \rightarrow \mathbb{C}$ is twice continuously differentiable complex-valued function and $w : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ a rapidly decreasing positive function.

Generalizing the analogous definitions of the last section, we agree on the following

Definition In analogy to (4.1.2) and (4.1.3), for any state ω with two-point correlation (4.2.1) we call

$$(1) \quad \rho_s(x) := \overline{q(x)} q(x)$$

the *density of the superfluid phase*,
and

$$(2) \quad \rho_n(x) := w(0)$$

the *density of the normal phase* in the state ω .

Using (2.3.3), we immediately calculate the (particle) *current density* of the superfluid in state ω , namely:

$$\mathbf{j}_s = \operatorname{Im}(\bar{q} \operatorname{grad} q), \quad (4.2.2)$$

where $\operatorname{grad} q$ denotes the complex gradient of q . The normal component represented by $w(x-y)$ obviously makes no contribution to the current and so we can meaningfully assign a hydrodynamic velocity field to the superfluid alone, defined on the complement of the set N of zeros of ρ_s . So we can continue the definition above by calling

$$(3) \quad \mathbf{v}_s(x) := \rho_s^{-1} \mathbf{j}_s \quad (4.2.3)$$

the *superflow* in the state ω .

Some interesting properties of the superflow $\mathbf{v}_s$, which have been postulated for a long time but have so far only been supported with less rigorous arguments, result directly from the following form of $\mathbf{v}_s$, which is verified with (4.2.2)

$$\mathbf{v}_s = \operatorname{Im}(q^{-1} \operatorname{grad} q). \quad (4.2.4)$$

In particular, $\mathbf{v}_s$ is irrotational in every simply connected open subset of its domain of definition $G = \mathbb{R}^3 \setminus N$ and has quantized circulation along every continuously differentiable closed path in G . This becomes evident in the most simple and elegant manner in Cartan's differential form calculus. The facts of interest in this context are summarized in the following lemma.

Lemma 4.2.1. Let $f : \mathbb{R}^n \rightarrow \mathbb{C}$ be a continuously differentiable function, N the set of zeros of f and $c : [a, b] \rightarrow \mathbb{R}^n$ a closed piecewise continuously differentiable path in $G := \mathbb{R}^3 \setminus N$. Then the following applies

(1) The differential form $\frac{df}{f}$ is closed in G (that is, its external derivative disappears).

$$(2) \quad \int_c \frac{df}{f} = 2\pi i I,$$

where $I \in \mathbb{Z}$ is the index of $0 \in \mathbb{C}$ of the path
 $c^* := f \circ c : [a, b] \rightarrow \mathbb{C}$.

Proof Ad (1): $d\left(\frac{df}{f}\right) = d\left(\frac{1}{f}\right) \wedge df = -\frac{1}{f^2} df \wedge df = 0$.

Ad (2): Verify that $\int_c \frac{df}{f} = \int_{c^*} \frac{dz}{z}$ and use Cauchy's integral formula. $\square$

Corollary (1) If $n = 3$:

$$\operatorname{rot}(f^{-1} \operatorname{grad} f) = 0 \quad \text{in } G.$$

$$(2) \quad \frac{1}{2\pi i} \int_c f^{-1} \operatorname{grad} f \, dx = I \in \mathbb{Z}. \quad (4.2.5)$$

This essentially implies the properties of $\mathbf{v}_s$ summarized in the next theorem.

Let the state ω still have the two-point function (4.2.1)

Main Theorem 4.2.2.

The superflow $\mathbf{v}_s$ in state ω is irrotational in G and has quantized circulation. In fact, for every closed piecewise continuously differentiable path $c : [a, b] \rightarrow G$ holds

$$\int_c \mathbf{v}_s \cdot d\mathbf{s} = 2\pi I,$$

where the *circulation number* $I \in \mathbb{Z}$ is the index of the path $c^* = q \circ c$ around $0 \in \mathbb{C}$.

The claim that a superflow $\mathbf{v}_s$ is irrotational is often derived from the more or less intuitive assumption that a hydrodynamic potential Θ should exist for $\mathbf{v}_s$ (cf. e.g. FEYNMAN [25], p. 335). The circulation of $\mathbf{v}_s$ then disappears in a simply connected volume, while it would be quantized in multiple connected domains. This idea is apparently wrong in this generality for the superflow $\mathbf{v}_s$ of the free Bose condensate (in general there is no potential for $\mathbf{v}_s$). Quantized vortices in convex vessel geometries were also observed *empirically* in helium II⁸. The relation $\mathbf{v}_s = \operatorname{grad} \Theta$ could therefore not apply globally, but had to be modified so that “cores” would appear in the superfluid, microscopic tubes in which there is no superfluid. Around such a core that destroys the simple connection of an area, the circulation of $\mathbf{v}_s$ could then be quantized. These ideas, developed largely ad hoc, now make sense in the case of a superflow $\mathbf{v}_s$ such as (4.2.4): From the main theorem above we see immediately that the circulation of $\mathbf{v}_s$ along c can only take on a value other than 0 if c is not C^1 -homologous to null in $G = \mathbb{R}^3 \setminus N$ (i.e. contractible in G to a point). Any compact C^1 -surface with boundary a closed curve c must therefore necessarily intersect the set N of zeros of ρ_s (i.e. figuratively “ c must go around N ”), if the circulation of $\mathbf{v}_s$ along c does not disappear, and for this to happen, $\mathbf{v}_s$ obviously has to become singular in N .

Every connected component of the set N in which ρ_s disappears can therefore be identified with a classical *core* of the superflow, as is done by the next definition.

Definition Let thus $N \subset \mathbb{R}^3$ denote the set where ρ_s vanishes and $G = \mathbb{R}^3 \setminus N$ its complement in $\mathbb{R}^3$. Since $\rho_s(x)$ is continuous, $N = \rho^{-1}(0)$ is closed in $\mathbb{R}^3$ and so G is an open subset of $\mathbb{R}^3$.

- (1) For each connected component V of N we call $(V, \mathbf{v}_s)$ a *quantized vortex with the core* V .

⁸ cf. RAYFIELD and REIF [43], PACKARD and SANDERS [16]. i Vortex quantization was also observed experimentally by VINEN [14], as well as by WHITMORE and ZIMMERMANN [15].

Definition (2) If $(V, \mathbf{v}_s)$ is a quantized vortex and $\mathcal{C}$ denotes the set of all null-homologous C^1 -cycles (i.e. the continuously differentiable contractible closed paths) in $G \cup V$ with positive circulation of $\mathbf{v}_s$, we define the *vortex strength* of $(V, \mathbf{v}_s)$ as

$$S := \inf_{c \in \mathcal{C}} \int_c \mathbf{v}_s \cdot d\mathbf{s} \quad .$$

If $\mathcal{C} = \emptyset$, then the vortex strength of $(V, \mathbf{v}_s)$ is said to be zero.

(3) If the core V of the vortex $(V, \mathbf{v}_s)$ is a one- or two-dimensional submanifold of $\mathbb{R}^3$, then V is called a *vortex line* or *vortex face*, respectively.

From (3.3.4) follows immediately in the two-liquid model an expression for the density of the *kinetic energy* in the superflow:

$$e_s := \text{diag} \frac{1}{2} (\nabla_x \cdot \nabla_y) \mathcal{W}_s(x, y) = \frac{1}{2} \|\text{grad } q\|^2 \quad (4.2.6)$$

where we set

$$\mathcal{W}_s(x, y) := \overline{q(x)} q(y) \quad .$$

The energy density (4.2.6) is higher than the 'energy density' calculated using the classical formula

$$e_{cl} = \frac{1}{2} \rho_s \mathbf{v}_s^2 \quad (4.2.7)$$

for the kinetic energy of a hydrodynamic flow $\mathbf{v}_s = \text{Im}(q^{-1} \text{grad } q)$. This follows directly from the inequality

$$\|\text{grad } q\| \geq \|\text{Im}(|q| q^{-1} \text{grad } q)\| \quad .$$

We consider (4.2.6) to be the correct (quantum dynamic) expression for the kinetic energy of the superflow and explain the difference to (4.2.7) by the fact that the classical idea, according to which arbitrarily small individualizable volumes of liquid move, fails here due to the Bose statistics. Particles may fluctuate in opposite directions within the liquid without this being macroscopically 'visible'.

We now return to the study of the *free* Bose gas. For as interesting as the class of states characterized by (4.2.6) is, insofar as they exhibit a flow $\mathbf{v}_s$ with some typical properties of a superfluid, such as long-range order and no rotation except at singularities in which the circulation is quantized, the fact is of course all the more interesting, that such states occur in the thermodynamic equilibrium of the free Bose gas.

Based on Lemma 3.3.1. it follows immediately from the foregoing that all KMS states of the free Bose gas with typical two-point correlation (4.1.1) exhibit a stationary superflow

$$\mathbf{v}_s = \text{Im}(Q^{-1} \text{grad } Q) \quad (4.2.8)$$

as characterized by Theorem 4.2.2.

Since Q is a Maxwell polynomial in this case, the kinetic energy of the superfluid contained in a compact volume $\Lambda \subset \mathbb{R}^3$, namely

$$U = \frac{1}{2} \int_{\Lambda} \|\text{grad } Q\|^2 dx \quad , \quad (4.2.9)$$

can also be expressed, using Green's first identity, by the surface integral

$$U = -\frac{1}{2} \int_{\partial\Lambda} \overline{Q} \partial Q \cdot dS \quad , \quad (4.2.10)$$

(where the surface $\partial\Lambda$ of Λ is assumed to be sufficiently smooth and ∂Q denotes the inner normal derivative on $\partial\Lambda$), a fact that will become interesting in view of the role of surface potentials for the formation of special vortex states. This will be discussed in Section 5.1.

To gain deeper insight into possible manifestations of superflow in the free Bose gas in the form of persistent currents and quantized vortices, we study specific examples of corresponding Bose condensed states in the next section.

4.3. Typical Examples

Below we are interested in special manifestations of superflow in the free Bose condensate. So according to the results of the last two sections, we have to consider superflows of the form

$$\mathbf{v}_s = \text{Im} (Q^{-1} \text{grad } Q) \quad , \quad (4.3.1)$$

where Q is any solution polynomial of the Laplace equation. We present some typical examples here and many more can be analogously constructed using general theorems on Maxwell polynomials; see e.g. [44]. The Examples (b) and (c) below were kindly provided to me by Professor Roepstorff. Since they are particularly illustrative, I am happy to accept his permission to include them here.

The most general Maxwell polynomial has the form

$$Q = \sum_{\substack{l=0 \\ -l \leq m \leq l}}^L c_l^m \mathcal{Y}_l^m \quad . \quad (4.3.2)$$

where $c_l^m \in \mathbb{C}$ and $\mathcal{Y}_l^m$ is the function

$$r^l Y_l^m(\theta, \phi) \quad (4.3.3)$$

transformed into Cartesian coordinates, Y_l^m denoting the spherical harmonics.

We recall that the gradient in spherical coordinates acts as the following differential operator

$$\mathbf{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \mathbf{e}_\theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin \theta} \mathbf{e}_\phi \frac{\partial}{\partial \phi} \quad (\nabla_{sph})$$

with

$$\begin{aligned}\mathbf{e}_r &:= \begin{pmatrix} \sin \theta \cos \phi, & \sin \theta \sin \phi, & \cos \theta \end{pmatrix} \\ \mathbf{e}_\theta &:= \begin{pmatrix} \cos \theta \cos \phi, & \cos \theta \sin \phi, & -\sin \theta \end{pmatrix} \\ \mathbf{e}_\phi &:= \begin{pmatrix} -\sin \phi, & \cos \phi, & 0 \end{pmatrix}\end{aligned}$$

(a) First we consider the case of a homogeneous harmonic polynomial

$$Q = \mathcal{Y}_l^m. \quad (4.3.4)$$

With this we get

$$\mathbf{v}_s(x, y, z) = \frac{m}{x^2 + y^2} (-y, x, 0). \quad (4.3.5)$$

This is seen by computing with the operator ∇_{sph} above

$$\begin{aligned}\mathbf{v}_s &= \mathcal{I}m(Q^{-1} \text{grad } Q) \\ &= \mathcal{I}m\left(\frac{l}{r} \mathbf{e}_r + \frac{1}{r \sin \theta} \left(\frac{a Y_{l+1}^m + b Y_{l-1}^m}{Y_l^m}\right) \mathbf{e}_\theta + i \frac{m}{r \sin \theta} \mathbf{e}_\phi\right) \\ &= \frac{m}{r \sin \theta} \mathbf{e}_\phi, \quad (*)\end{aligned}$$

where we have used

$$\frac{\partial}{\partial \theta} Y_l^m = \frac{1}{\sin \theta} \left(\underbrace{\frac{l(l+1)}{[(2l+1)(2l+3)]^{1/2}}}_{a} Y_{l+1}^m - \underbrace{\frac{l(l+1)}{[(2l-1)(2l+1)]^{1/2}}}_{b} Y_{l-1}^m \right),$$

see e.g. EDMONDS [45], p. 79.

The expression (*) transformed into Cartesian coordinates gives (4.3.5).

As this expression directly displays, $\mathbf{v}_s$ circulates concentrically around the z-axis and has a singularity there, which is the connected set of zeros of $Q = \mathcal{Y}_l^m$ and the core of a vortex of strength $2\pi|m|$. So in the simplest non-trivial case

$$Q = x + iy \quad (4.3.6)$$

we get a vortex line in the z-axis of strength 2π , cf. figure 2 on page 31.

(b) Closed vortex lines

These are also typical manifestations of superflow in the Bose condensate.

To construct such vortices, we consider a class of Maxwell polynomials Q with axial symmetry around the z-axis. For every such polynomial, in the representation (4.3.2) the factor c_l^m must always be zero whenever $m \neq 0$. This follows immediately from

$$\frac{\partial}{\partial \phi} \tilde{Q} = 0$$

and from the linear independence of the $r^l Y_l^m$, with $\tilde{Q}$ denoting Q transformed into spherical coordinates.

Therefore Q allows a representation in the form

$$Q = \sum_{l=0}^L a_l r^l P_l(z/r) \quad \text{with} \quad r^2 := x^2 + y^2 + z^2$$

in which P_l denotes the l -th Legendre polynomial. With a suitable choice of the coefficients a_l there exist $a, R_1, \dots, R_m \in \mathbb{R} \setminus \{0\}$ such that with $a_1 := ia$

$$\sum_{l=0}^L a_l \rho^l P_l(a) = a \prod_{\mu=1}^m (\rho^2 - R_\mu^2) \quad \text{with} \quad \rho^2 := x^2 + y^2$$

(note that $P_{2\nu+1}(0) = 0$ for all $\nu \in \mathbb{N}$).

Then $\mathbf{v}_s$ becomes singular in the $z = 0$ plane along the circles

$$\rho^2 = R_\mu^2 \quad .$$

An example of a circular vortex line of strength π is given with

$$Q = x^2 + y^2 - 2z^2 + iz - R^2 \quad , \quad (4.3.7)$$

in which case we calculate the circulation 2π along the path

$$\begin{aligned} c : [0, 2\pi] &\longrightarrow \mathbb{R}^3 \\ \psi &\longmapsto (0, R(1 + \cos \psi), R \sin \psi) \end{aligned}$$

The following figure shows the flow lines of this vortex in a section along the z -axis.

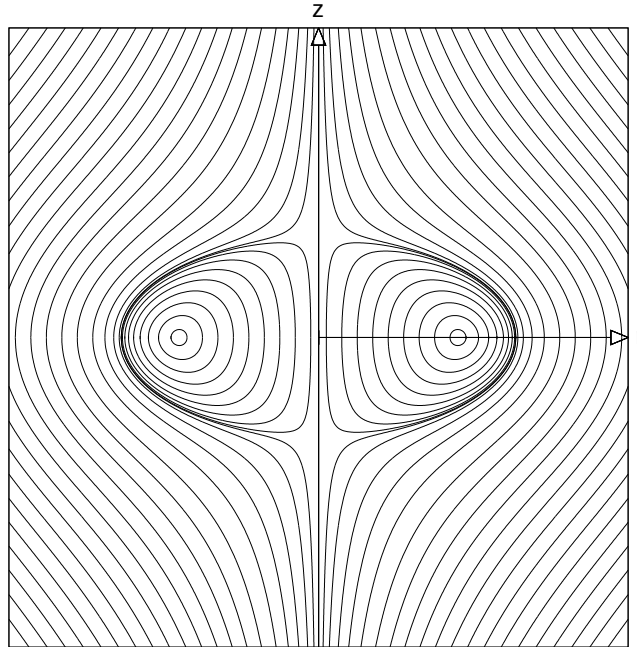


Fig. 3. Flow lines of the velocity field $\mathbf{v}_s = \mathcal{I}m(Q^{-1}\nabla Q)$ for Q in (4.3.7).

(c) Two-dimensional flows

We restrict ourselves to Maxwell polynomials, which, like the simple example (4.3.6), depend of only two variables x and y , which are identified with the complex number $z = x + iy$.

In $\mathbb{C}$ the Maxwell equation is

$$\frac{\partial}{\partial z \partial \bar{z}} Q(z) = 0, \quad (4.3.8)$$

from which it immediately follows that all holomorphic and antiholomorphic functions are harmonic. Thus, especially the functions

$$\begin{aligned} & a(z - a_1)(z - a_2) \cdots (z - a_n) \\ \text{and} \quad & a(\overline{z - a_1}) \overline{(z - a_2)} \cdots \overline{(z - a_n)}. \end{aligned} \quad (4.3.9)$$

For $\mathbf{u} := \mathbf{v}_{s_1} - i\mathbf{v}_{s_2}$ we then get, respectively,

$$\mathbf{u} = -i \sum_{\nu=1}^n \frac{1}{z - a_\nu} \quad \text{and} \quad \mathbf{u} = i \sum_{\nu=1}^n \frac{1}{z - a_\nu}.$$

Along any closed, positively oriented C^1 -path c in the complement of the set of zeros $\{a_1, \dots, a_n\}$, the circulation

$$\int_c \mathbf{v}_s \cdot d\mathbf{s} = \int_c \mathbf{u} dz$$

is always a positive in the first case and always negative in the second case.

So something like the following pictures might appear in the corresponding cases

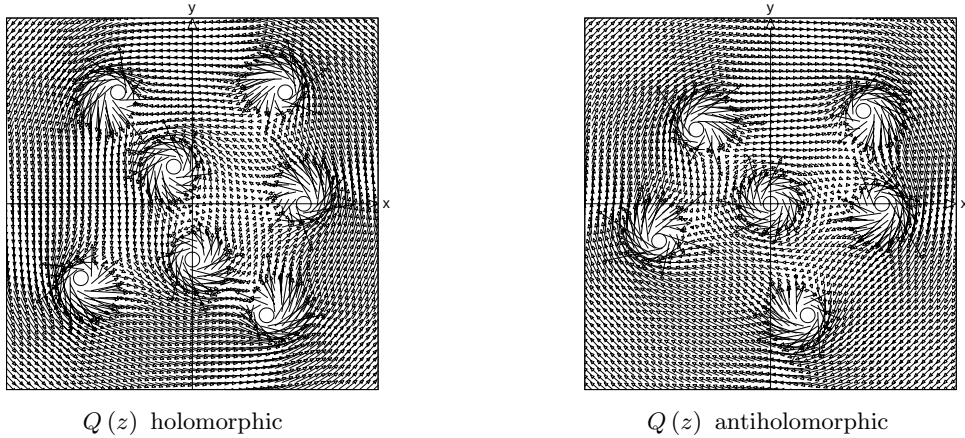


Fig. 4. Vortices for holomorphic and antiholomorphic Q as in (4.3.9). In the vortex centers, the velocity $\mathbf{v}_s$ becomes singular of order $1/r$, r being the distance from the center. This is illustrated in Fig.1., page 10, for the holomorphic case.

5. The Thermodynamic Limit

5.1. Boundary and Environment

In the quantum mechanical description of an otherwise free particle in a compact volume Λ with a smooth boundary $\partial\Lambda$, it makes sense to simulate certain surface potentials using the boundary conditions which have to be imposed on the Laplace differential operator in order to obtain an energy spectrum - i.e. mathematically, in order to ensure the *self-adjointness* of the Laplacian in $L^2(\Lambda)$. ROBINSON [11] proposes a classification of the following 'self-adjoint' boundary conditions

$$\partial\phi = p\phi \quad (*)$$

in terms of surface behavior ($\partial\phi$ denotes the inner normal derivative of any smooth function ϕ and p a measurable real function defined on the boundary surface $\partial\Lambda$). In areas with vanishing p he ascribes to the surface an ideally reflective behavior, while areas with negative or positive p correspond to an attractive, respectively repulsive, behavior of the surface. Consistent with that, the spatial density of an otherwise free particle in the ground state of the Hamiltonian $h_0 = -\frac{1}{2}\Delta$ decreases from the boundary or increases, to the extent imposed by p . This is also reflected in the behavior of the eigenvalues. For an everywhere negative, respectively positive p , the spectrum of h_0 has a negative or positive lower bound. In the first case, this can be understood as a binding of the associated eigenstates to the attractive surface potential p (as e.g. ROBINSON interprets it in [10]), and in the second case as an increase in their energy levels through the repulsive boundary potential.

With $C^\infty(\mathbb{R}^n)$, the space of all complex-valued C^∞ -functions in $\mathbb{R}^n$, we define for any compact volume $\Lambda \subset \mathbb{R}^n$ with smooth boundary $\partial\Lambda$ the prehilbert subspace $\mathcal{D}(\Lambda) \hookrightarrow L^2(\Lambda)$ as the $\mathbb{C}$ -linear span of all $\{\phi \upharpoonright \Lambda \mid \phi \in C^\infty(\mathbb{R}^n)\}$ (observe that the functions of $\mathcal{D}(\Lambda)$ generally do not vanish on $\partial\Lambda$, due to the truncation ' $\upharpoonright$ ').

If especially p is a continuous function on the border $\partial\Lambda$ of a compact smoothly bordered C^∞ -submanifold $\Lambda \hookrightarrow \mathbb{R}^3$, then the quadratic form on $\mathcal{D}(\Lambda)$

$$q(u) := \frac{1}{2} \int_{\partial\Lambda} p \bar{u}_\circ u_\circ dS \quad (**)$$

(which is continuous on $H_1(\Lambda) \subset L^2(\Lambda)$ by the Trace Theorem; see Appendix, p. 65) is given the physical interpretation of the *surface energy in the state u* . Note that $u_\circ$ in the above expression represents the image of u under the canonical mapping from $\mathcal{D}(\Lambda)$ to $\mathcal{D}(\partial\Lambda)$ continuously extended to a map from $H_1(\Lambda)$ into $H_{\frac{1}{2}}(\partial\Lambda)$ (see the Trace Theorem, p. 65).

The factor 1/2 in (**) is suggested by Green's first identity and especially (4.2.9), (4.2.10), which ensure that with the attractive boundary conditions (5.1.1) for $h_0 = -1/2\Delta$ and the expectation value of the energy of a particle in state u , i.e.

$$\langle h_0 u, u \rangle = \frac{1}{2} \int_{\Lambda} \|\text{grad } u\|^2 dx + q(u),$$

the kinetic energy of the supercurrent equals its potential energy at the boundary (which is shifted to infinity in the thermodynamic limit, cf. Theorem 5.1.5.).

In this interpretation, the above terms $\frac{1}{2} \int_{\Lambda} \|\text{grad } u\|^2 dx$ and $q(u)$ represent, respectively, the expected values of the kinetic and potential energy of a particle in state u under the influence of an attractive boundary $\partial\Lambda$.

If one considers a *grand canonical* quantum system in a compact volume (that is, a spatially finite quantum system in a *Gibbs state*) the quantum mechanical boundary conditions imposed by the surface potential p are complemented by the thermodynamic boundary conditions, which characterize a certain environmental contact in equilibrium, in particular temperature and chemical potential ('heat bath' and 'particle reservoir'). It is of course a gross simplification to describe the entire thermodynamic contact of a system with its environment by just two parameters. Many forms of contact between a system and its environment (particularly with its boundary) do not fit into this simple scheme. Consider, for example, the possibility that certain states are preferentially created or destroyed at the surface. Such an effect would correspond to that of a catalyst. It could be exploited to separate different state components (such as in a process to separate ortho- and para-hydrogen by exploiting higher concentrations of one component near a metallic surface). At least in this case a grand canonical description would still be possible by making the chemical potential state-dependent.

In the following we will introduce boundary conditions for the one-particle Hamiltonian of the free Bose gas, which, together with a splitting of the chemical potential, generate some of the KMS states described in Chapter 4 in the limit of the infinitely extended system. Simply put, the surface removes some of the states, causing macroscopic population at a higher level. The mechanism corresponds to that described by ROBINSON [10]: In the thermodynamic limit, phase separation occurs whereby under the influence of attractive boundary conditions (imposed on the Laplacian), the 'surface-bound' states condense earlier and flow out of the bulk.

The boundary conditions for the Laplace operator determine quantum mechanically the microscopic dynamics of the single non-interacting Bose particles. We impose the following.

The boundary conditions : Let $\Lambda \subset \mathbb{R}^3$ be a bordered compact C^∞ -submanifold of $\mathbb{R}^3$, star-shaped with respect to the inner point $0 \in \mathbb{R}^3$ (otherwise said, Λ is a compact volume with a smooth surface and such that every ray emanating from the origin hits this surface exactly once). Furthermore, let Q be a harmonic polynomial in $\mathbb{R}^3$, homogeneous of degree $l \in \mathbb{N}$, such that $Q^{-1}\partial Q$ is real and bounded on $\partial\Lambda$ (∂Q denotes the derivative of Q in the direction of the inner surface normal).⁹ Also, let Q be normalized in $L^2(\Lambda)$.

For $R > 0$ we define

$$\Lambda_R := \{x \mid R^{-1}x \in \Lambda\} \quad \text{and} \quad \mathcal{H} := L^2(\Lambda_R).$$

Then, according to Theorem A.4. in the Appendix (cf. p. 63), the Laplace operator Δ exists and is self-adjoint in $\mathcal{H}$ under the boundary conditions

$$Q \partial \phi = \phi \partial Q \quad \text{on} \quad \partial\Lambda_R \tag{5.1.1}$$

and Q is eigenvector of Δ with eigenvalue zero.

⁹ All requirements are fulfilled, for example, for any homogeneous polynomial Q of degree l and $\Lambda = B^3$. Then obviously $Q^{-1}\partial Q = -l$ on $\partial\Lambda = S^2$.

The spectrum of $h_0 = -\frac{1}{2}\Delta$ is discrete and bounded below by a generally *negative* lower bound (cf. Appendix, Theorem A.5., p. 64). In the sense of the introductory remarks of this section, we therefore speak of 'attractive' boundary conditions for h_0 .

We consider all positive eigenstates of h_0 to be 'free', all negative ones to be 'bound to the surface'. More precisely, all states are said to be bound to the surface that disappear from the system in the limit $R \rightarrow \infty$ under conditions for the chemical potential to be further specified below.

Definition The boundary conditions (5.1.1) still apply. We define the subspace $\mathcal{P} \subset \mathcal{H}$ spanned by Q and all positive eigenvectors of h_0 (that is, those with positive eigenvalues) as the space of *free* single-particle states in $\mathcal{H}$. Its projector is written P .

Accordingly, we call the subspace $\mathcal{N} := \mathcal{P}^\perp$ with pertinent projector N into the span of all negative eigenvectors of h_0 the space of all single-particle states *bound to the surface* or border of Λ_R .

The binding of some states to the border is also expressed in the chemical potential μ_R by allowing a function of P and N instead of just a multiple of the identity of $\mathcal{H}$. Accordingly, the one-particle Hamiltonian is defined as

$$h := -\frac{1}{2}\Delta - \mu_R, \quad (5.1.2)$$

where Δ is the Laplacian with boundary conditions (5.1.1) and $\mu_R := \mu_1 N + \mu_2 P$ with $\mu_1, \mu_2 \in \mathbb{R}_+$ is the R dependent operator of the chemical potential.

The description of the quantum *system* is now canonical, namely the Bose gas in the volume Λ_R with dynamics induced by h is the quasi-free dynamical system $(\mathfrak{W}, \alpha)$, consisting of the Weyl algebra $\mathfrak{W}$ over $\mathcal{H} = L^2(\Lambda_R)$ and the one-parameter group α of $*$ -automorphisms of $\mathfrak{W}(\mathcal{H})$ induced by the operation of e^{ih} in $\mathcal{H}$, that is

$$\alpha_t W(u) = W(e^{ith} u), \quad u \in \mathcal{H}.$$

In the Fock representation of $\mathfrak{W}(\mathcal{H})$ in the symmetric Fock space $\mathcal{F}(\mathcal{H})$, α is generated by the second quantization H of h :

$$e^{-itH} W_{\mathcal{F}}(u) e^{itH} = W_{\mathcal{F}}(e^{ith} u).$$

It is known that for $h > 0$ (which can always be achieved by a suitable choice of the chemical potential μ_R , because $h_0 = -\frac{1}{2}\Delta$ is bounded from below) there exists exactly one extremal KMS state ω_R for the dynamics α and inverse temperature β , namely the grand canonical Gibbs state, which in the Fock representation is given by the density operator

$$\Gamma = e^{-\beta H} / \text{Tr } e^{-\beta H} \quad (5.1.3)$$

on the symmetric Fock space $\mathcal{F}(\mathcal{H})$.

The generating functional of this state is calculated in the canonical manner as

$$E^R(u) = \text{Tr } \Gamma W_{\mathcal{F}}(u) = \exp\left(-\frac{1}{4} \langle u, \coth\left(\frac{\beta h}{2}\right) u \rangle\right). \quad (5.1.4)$$

By separating in $\mathcal{H} = L^2(\Lambda)$ the single-particle states into free ones and those that are bound to the surface, the entire system in a KMS state is split into two subsystems in thermodynamic equilibrium. The following theorem provides the mathematical basis of this splitting.

Theorem 5.1.1. Let $\mathcal{K}$ be a Hilbert space.

- (1) Every direct sum decomposition

$$\mathcal{K} = \mathcal{K}_1 \oplus \mathcal{K}_2$$

induces an isomorphism $\cong$ of the symmetric Fock spaces

$$\mathcal{F}(\mathcal{K}) \cong \mathcal{F}(\mathcal{K}_1) \otimes \mathcal{F}(\mathcal{K}_2),$$

which is uniquely defined by the functorial connection

$$(v \oplus w)^\sim \cong v^\sim \otimes w^\sim.$$

where for $u \in \mathcal{K}$ the associated *coherent* state (or 'Glauber' state) in the symmetric Fock space $\mathcal{F}(\mathcal{K})$ is written as $u^\sim$.¹⁰

- (2) Let $\mathcal{K} = \mathcal{K}_1 \oplus \mathcal{K}_2$ and h be a positive self-adjoint operator in $\mathcal{K}$ that is reduced by $\mathcal{K}_1$ and $\mathcal{K}_2$, i.e. $h = h_1 \oplus h_2$. Also let $h^\sim$ denote the second quantization of h , uniquely defined by

$$e^{ith^\sim} u^\sim = (e^{ith} u)^\sim$$

then for all $z \in \mathbb{C}$ with $\text{Re } z \leq 0$

$$e^{zh^\sim} \cong e^{zh_1^\sim} \otimes e^{zh_2^\sim}.$$

Proof

Ad (1): See DAVIES [46], Chapter 8, p. 119.

Ad (2): Denote the self-adjoint generators of the unitary 1-parameter groups

$$e^{ith_1^\sim} \otimes \mathbf{1} \quad \text{and} \quad \mathbf{1} \otimes e^{ih_2^\sim}, \quad \text{respectively,}$$

as

$$h_1^\sim \otimes \mathbf{1} \quad \text{and} \quad \mathbf{1} \otimes h_2^\sim.$$

Then the spectral families $E_\lambda \otimes \mathbf{1}$ and $\mathbf{1} \otimes F_\lambda$, where E_λ and F_λ are the spectral families of $h_1^\sim$ and $h_2^\sim$, respectively, obviously commute. Therefore, according to von Neumann's theorem (cf. RIESZ & NAGY [47], p. 358), a self-adjoint operator S exists in $\mathcal{F}(\mathcal{K}_1) \otimes \mathcal{F}(\mathcal{K}_2)$, such that with real Borel measurable functions f and g on the spectrum of S

$$h_1^\sim \otimes \mathbf{1} = f(S) \quad \text{and} \quad \mathbf{1} \otimes h_2^\sim = g(S).$$

¹⁰ For every $u \in \mathcal{K}$ the state $u^\sim \in \mathcal{F}(\mathcal{K})$ is uniquely defined by its components in the n -particle subspaces of $\mathcal{F}(\mathcal{K})$, namely

$$(u^\sim)_n := (n!)^{-\frac{1}{2}} e^{-\|u\|^2/2} \otimes^n u.$$

This $u^\sim$ is called the *coherent state* or also the *Glauber state* associated to u .

Since with f and g their sum is also Borel measurable on the spectrum of S , the self-adjoint operator

$$H := (f + g)(S)$$

exists and is unique and

$$H \subseteq h_1^\sim \otimes \mathbf{1} + \mathbf{1} \otimes h_2^\sim .$$

In the operator functional calculus (cf. RIESZ and NAGY [47], section 128) follows

$$\begin{aligned} e^{zH} &= e^{z(f+g)(S)} = e^{zf} e^{zg}(S) = e^{zf(S)} e^{zg(S)} \\ &= (e^{zh_1^\sim \otimes \mathbf{1}})(e^{z\mathbf{1} \otimes h_2^\sim}) = e^{zh_1^\sim} \otimes e^{zh_2^\sim} . \end{aligned} \quad (*)$$

Therefore all that remains to be shown is that $h^\sim = H$, which is clearly the case if

$$e^{ith^\sim} \cong e^{itH} , \quad \text{for all } t \in \mathbb{R} .$$

Since the coherent states span the symmetric Fock space, we can proceed like this

$$\begin{aligned} e^{ith^\sim}(v \oplus w)^\sim &= (e^{ith_1} v \oplus e^{ith_2} w)^\sim \cong (e^{ith_1} v)^\sim \otimes (e^{ith_2} w)^\sim \\ &= (e^{ith_1^\sim} v^\sim) \otimes (e^{ith_2^\sim} w^\sim) = (e^{ith_1^\sim} \otimes e^{ith_2^\sim})(v^\sim \otimes w^\sim) \\ &= e^{itH}(v^\sim \otimes w^\sim) . \end{aligned}$$

□

Conclusion If h is the one-particle Hamiltonian in $\mathcal{H}$ given by (5.1.2), $h > 0$ and H is the second quantization of h in $\mathcal{F}(\mathcal{H})$, then the grand canonical Gibbs state Γ (cf. (5.1.3)) factorizes in $\mathcal{F}(\mathcal{H}) \cong \mathcal{F}(\mathcal{P}) \otimes \mathcal{F}(\mathcal{N})$ into the Gibbs states of the free and the surface-bound components, respectively represented by $\mathcal{F}(\mathcal{P})$ and $\mathcal{F}(\mathcal{N})$, that is, explicitly

$$e^{-\beta H} / Tr \cong e^{-\beta h P} / Tr_1 \otimes e^{-\beta h N} / Tr_2 .$$

(Tr and Tr_ν respectively denote the trace of the operator in the numerator.)

In the thermodynamic limit we shall impose three constraints (UNI), (POS) and (CON) on the R -dependent operator $\mu_R = \mu_1 N + \mu_2 P$ of the chemical potential defined in (5.1.2), or equivalently on the *fugacity* operator $z_R = e^{\beta \mu_R}$, which must be met for all $R > 0$. On the one hand, (UNI) ensures that μ_R becomes uniform in the thermodynamic limit (which reflects the disappearance of the boundary influence in the infinitely extended system). On the other hand (POS) ensures the positivity of h and thus the thermodynamic stability, i.e. the existence of the grand canonical state Γ , cf. (5.1.3). Finally, (CON) causes the targeted Bose condensation with simultaneous convergence of the local particle density.

We generally specify that μ_R should be a negative function of P and $N = P^\perp$. Since in general $h_0 = -\frac{1}{2}\Delta$ with the boundary conditions (5.1.1) also has negative eigenvalues, this requirement alone is not sufficient to ensure the positivity of h as defined in (5.1.2).

However, positivity of h is guaranteed if the following condition is imposed on μ_R

$$(\text{POS}) \quad R^2 \mu_R \upharpoonright \mathcal{N} \leq C \quad ,$$

where C is a constant smaller than the lower bound of the spectrum of $-\frac{1}{2}\Delta$ for $R = 1$.

The second condition is

$$(\text{UNI}) \quad \lim_{R \rightarrow \infty} \mathbf{z}_R = \zeta \mathbf{1} \quad , \quad \text{with} \quad \zeta := e^{\beta\mu} \in (0, 1] \quad ,$$

where the convergence is to be understood as norm convergence in $\mathcal{B}(L^2(\mathbb{R}^3))$ and $L^2(\Lambda_R)$ as a subspace of $L^2(\mathbb{R}^3)$.

Finally, with l denoting the degree of the homogeneous polynomial Q in (5.1.1)

$$(\text{CON}) \quad \lim_{R \rightarrow \infty} \mathbf{z}_R (\mathbf{1} - \mathbf{z}_R)^{-1} R^{-3-2l} = c \mathbf{1} \quad , \quad \text{for any } c \in [0, \infty) \quad ,$$

in norm convergence (and hence all the more weak convergence on $L^2(\mathbb{R}^3)$).

So if we write $\mathbf{z}_R$ as $z_1 P + z_2 N$ then (UNI) says that z_1 and z_2 both must converge to $\zeta = e^{\beta\mu}$ and (CON) says that thereby $z_1 (1 - z_1)^{-1} R^{-3-2l}$ converges to c . The comparison of (UNI) and (CON) also shows that necessarily

$$c = 0 \quad \text{if} \quad \zeta < 1 \quad .$$

Main Theorem 5.1.2.

Under the boundary conditions (5.1.1), let $h = -\frac{1}{2}\Delta - \mu_R$ and E^R be defined as in (5.1.2) and (5.1.4).

If (POS), (UNI) and (CON) are met, then the following applies

- (1) E^R converges simply on $\mathcal{S}(\mathbb{R}^3)$ against the generating functional

$$E(u) = \exp\left(-\frac{1}{2}c|Q[u]|^2\right) E_\zeta(u) \quad , \quad u \in \mathcal{S}(\mathbb{R}^3)$$

(so necessarily $c = 0$ if $\zeta < 1$; E_ζ as in (3.3.1)).

E is therefore the generating functional of a quasi-free, hence in particular gauge invariant state ω on $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ with the two-point function

$$\mathcal{W}(x, y) = c \overline{Q(x)} Q(y) + w_\zeta(x - y)$$

- (2) The state ω extends continuously (in the sense of Lemma 2.2.1.) to a state on the tempered Weyl algebra, which is β -KMS with respect to the free dynamics α (cf. p. 21, Def. (3)) with $\zeta = e^{\beta\mu}$.

Main Theorem 5.1.2.

(cont'd)

$$(3) \quad \lim_{R \rightarrow \infty} n_{\mathcal{V}}(R) = c \int_{\mathcal{V}} \overline{Q} Q \, dx + V w_{\zeta}(0) .$$

Thus, for every (fixed) bounded volume $\mathcal{V} \subset \mathbb{R}^3$, when R approaches infinity, the mean particle density in $\mathcal{V}$ of the states ω_R becomes identical to the mean particle number in $\mathcal{V}$ of the state ω . (That is, the thermodynamic limit and the reduction of the limit state to a local mean particle density are interchangeable).

Corollary to (3) (Existence of a critical density)

Condensation ($c \neq 0$) occurs under the assumptions of the above theorem if and only if in every given compact $\mathcal{V} \subset \mathbb{R}^3$ with non-vanishing volume the mean density in the limit $R \rightarrow \infty$ approaches a value above the *critical density*

$$w_1(0) = (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(1) . \quad (5.1.5)$$

The special case with $Q = \text{const}$, i.e. $l = 0$ and $\mathcal{N} = \emptyset$, obviously yields the 'classical' Bose-Einstein condensate with isotropic and translation-invariant density.

Proof We apply a method first used by LEWIS and PULÉ [6] that is based on estimates for the Greens function of the heat equation, which were originally inspired, as they note, by a private communication from MARK KAC.

Let $-\frac{1}{2}\Delta$ be the self-adjoint operator in $L^2(\Lambda_R)$ with the boundary conditions (5.1.1) and let its eigenvalues be

$$\varepsilon_0^R < \varepsilon_1^R \leq \dots \leq \varepsilon_L^R < \varepsilon_{L+1}^R \leq \dots \quad (A)$$

listed with their multiplicities. Furthermore, let

$$\{e_k^R\}_{k \in \mathbb{N}} \quad \text{with} \quad e_k^R(x) := R^{-\frac{3}{2}} e_k^1(R^{-1}x) \quad (B)$$

be an associated orthonormal basis for $L^2(\Lambda_R)$ corresponding to the eigenvalues (A) with $e_L^1 = Q$. Remember, Q was assumed to be normalized in $L^2(\Lambda)$, therefore $e_L^R(x) = R^{-\frac{3}{2}} e_L^1(R^{-1}x) = R^{-\frac{3}{2}-l} Q(x)$ is normalized in $L^2(\Lambda_R)$. Then

$$G^R(x, y, t) = \sum_{k \in \mathbb{N}} \exp(-t \varepsilon_k^R) \overline{e_k^R(x)} e_k^R(y)$$

is the Greens function of the heat equation

$$\frac{\partial}{\partial t} \phi = -\frac{1}{2} \Delta \phi$$

in $\Lambda_R \times \mathbb{R}_+$ with the same boundary conditions (5.1.1).

A known fundamental solution of the heat equation in $\mathbb{R}^3 \times \mathbb{R}_+$ is

$$G_F^R(x, y, t) = (2\pi t)^{-\frac{3}{2}} \exp\left(-\frac{|x-y|^2}{2t}\right).$$

For $L \in \mathbb{N}$ and $u \in \mathcal{D}(\mathbb{R}^3)$ we define

$$\text{and} \quad \left. \begin{aligned} K_R(s) &:= \sum_{k=L+1}^{\infty} \exp(-s\varepsilon_k^R) | \langle \mathbf{e}_k^R, u \rangle |^2 \\ K(s) &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} G_F^R(x, y, s) u(x) \overline{u(y)} dx dy \end{aligned} \right\} \quad (5.1.6)$$

With these functions the following applies.

Lemma 5.1.3. (LEWIS & PULÉ)

If $f : \mathbb{R}_+ \mapsto [0, 1]$ is any function, then this implication is correct

$$\lim_{R \rightarrow \infty} f(R) = \zeta \implies \lim_{R \rightarrow \infty} \sum_{n=1}^{\infty} f^n(R) K_R(n\beta) = \sum_{n=1}^{\infty} \zeta^n K(n\beta)$$

One verifies that the series on the right equals $\langle w_\zeta * u, u \rangle$, see (3.3.1).

Proof of the Lemma

The above statement is a slight generalization of Lemma 2 by LEWIS and PULÉ [6], which concerns the special case $L = 0$. The proof in [6] is reduced to the following inequality (C) which holds for any $L > 0$.

For every $t \in \mathbb{R}_+$ there exists a $c(t) \in \mathbb{R}_+$ so that for all natural numbers with $n < tR^2/\beta$ holds

$$|K_R(n\beta) - K(n\beta)| < c(t) R^{-\frac{1}{2}} n^{-\frac{5}{4}}. \quad (C)$$

We essentially recapitulate the proof of (C) from [6] with the completions necessary for the case $L > 0$.

With $G_C^R := G^R - G_F^R$ and the above definitions of K and K_R , see (5.1.6), obviously holds

$$\begin{aligned} K_R(n\beta) &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} G_C^R(x, y, n\beta) u(x) \overline{u(y)} dx dy + K(n\beta) \\ &\quad - \sum_{k=0}^L \exp(-n\beta \varepsilon_k^R) | \langle \mathbf{e}_k^R, u \rangle |^2. \end{aligned}$$

From the asymptotic behavior of the eigenvalues ε_k^R , see Appendix, Theorem A.5., it follows that the series G^R converges uniformly and can therefore be integrated term by term.

It follows from the last equation that

$$\begin{aligned} |K_R(n\beta) - K(n\beta)| &\leq \left| \int_{\mathbb{R}^3 \times \mathbb{R}^3} G_C^R(x, y, n\beta) u(x) \overline{u(y)} dx dy \right| + \\ &+ \sum_{k=0}^L \exp(-n\beta \varepsilon_k^R) | \langle \mathbf{e}_k^R, u \rangle |^2. \end{aligned}$$

Due to (B), for a certain constant C_0 the last sum remains less than $R^{-3} e^{-t\varepsilon_0^1} C_0$ if $n < tR^2/\beta$ (here was used $\varepsilon_k^R = R^{-2}\varepsilon_k^1$).

Therefore, for $n < tR^2/\beta$ the sum is less than

$$\begin{aligned} R^{-3} e^{-\varepsilon_0^1} C_0 &= R^{-\frac{1}{2}} R^{-\frac{5}{2}} e^{-t\varepsilon_0^1} C_0 < R^{-\frac{1}{2}} (t\beta)^{-\frac{5}{4}} e^{-t\varepsilon_0^1} n^{-\frac{5}{4}} C_0. \\ &(\text{ } \uparrow \text{ } n < tR^2/\beta) \end{aligned}$$

So with

$$c_1(t) := (t\beta)^{-\frac{5}{4}} e^{-t\varepsilon_0^1} C_0$$

the sum is less than $c_1(t) R^{-\frac{1}{2}} n^{-\frac{5}{4}}$ whenever $n < tR^2/\beta$. (D)

Theorem A.5 yields for $R^{-2}n\beta < t$ and a certain constant $c_2(t)$

$$|G_C^R(x, y, n\beta)| = R^{-3} |G_C^1(R^{-1}x, R^{-1}y, R^{-2}n\beta)| < (n\beta)^{-\frac{3}{2}} e^{-l_y \frac{R^2}{2n\beta}} c_2(t)$$

where

$$l_y := \inf_{y \in \Lambda_{R_0}} \text{dist}(R^{-1}y, \partial\Lambda) = \inf_{y \in \Lambda_{R_0/R}} \text{dist}(y, \partial\Lambda) = \text{dist}(\Lambda_{R_0/R}, \partial\Lambda)$$

Choose R_0 so large that the support of u is in Λ_{R_0} (such an R_0 exists, since $u \in \mathcal{D}(\mathbb{R}^3)$).

If then $R \geq 2R_0$, i.e. $l_y \geq \text{dist}(\Lambda_{\frac{1}{2}}, \partial\Lambda)$, it follows that for a certain $C(t)$ holds

$$|G_C^R(x, y, n\beta)| < (n\beta)^{-\frac{3}{2}} \left(\frac{n\beta}{2l_y R^2} \right)^{\frac{1}{4}} C(t) =: c_3(t) R^{-\frac{1}{2}} n^{-\frac{5}{4}}, \quad (\text{E})$$

whenever $n < tR^2/\beta$.

So for a sufficiently large R and all natural numbers $n < tR^2/\beta$ applies

$$|K_R(n\beta) - K(n\beta)| < (c_1(t) + |\hat{u}(0)|^2 c_3(t)) R^{-\frac{1}{2}} n^{-\frac{5}{4}} =: c(t) R^{-\frac{1}{2}} n^{-\frac{5}{4}}.$$

Since $K_R(s) - K(s)$ is a continuous function of $(R, s) \in \mathbb{R}_+ \times \mathbb{R}_+$, such a $c(t)$ exists for all $R > 1$, i.e. (C) applies.

From (C) and $\lim_{R \rightarrow \infty} f(R) = \zeta \in [0, 1]$ one now concludes that

$$\lim_{R \rightarrow \infty} \left| \sum_{n=1}^{\infty} f^n(R) K_R(n\beta) - \sum_{n=1}^{\infty} \zeta^n K(n\beta) \right| = 0$$

(see estimates I, II, III in the proof of Lemma 2 in [6]).

□

Remark The proof of the lemma can be translated almost literally into the proof of the statement that is obtained if $K_R(n\beta)$ and $K(n\beta)$ in Lemma 5.1.3 are replaced with

$$K'_R(n\beta) := \sum_{k=L+1}^{\infty} \exp(-n\beta\varepsilon_k^R) \int_{\mathcal{V}} |\mathbf{e}_k^R(x)|^2 dx$$

and

$$K'(n\beta) := \int_{\mathcal{V}} G_F^R(x, y, n\beta) dx ,$$

respectively .

The statement then reads:

Lemma 5.1.4. Let $f : \mathbb{R}_+ \mapsto [0, 1]$ any function. Then

$$\lim_{R \rightarrow \infty} f(R) = \zeta \implies \lim_{R \rightarrow \infty} \sum_{n=1}^{\infty} f^n(R) K'_R(n\beta) = \sum_{n=1}^{\infty} \zeta^n K'(n\beta) .$$

Comparison with (3.3.1) shows that the last series equals

$$V w_{\zeta}(0) = V (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(\zeta) , \text{ with } V = \text{Vol}(\mathcal{V}) .$$

Now back to the proof of the Theorem 5.1.2.

Ad (1): We obtain for $E^R(u)$, see (5.1.4),

$$E^R(u) = \exp\left(-\frac{1}{4} \|u\|^2\right) \exp\left(-\frac{1}{2} (u, u)_R\right) ,$$

with

$$\begin{aligned} (u, u)_R &= \sum_{k=0}^{L-1} (\exp(\beta(\varepsilon_k^R - \mu_1)) - 1)^{-1} |\langle \mathbf{e}_k^R, u \rangle|^2 \\ &\quad + \sum_{k=L}^{\infty} (\exp(\beta(\varepsilon_k^R - \mu_2)) - 1)^{-1} |\langle \mathbf{e}_k^R, u \rangle|^2 \end{aligned}$$

where $\boldsymbol{\mu} = \mu_1 N + \mu_2 P$, $\mu_{\nu} = \mu_{\nu}(R)$.

(POS) implies that

$$R^2 \mu_1 \leq C \leq \varepsilon_0^1 ,$$

from which follows for $k < L$

$$\begin{aligned} 0 &< (\exp(\beta(\varepsilon_k^R - \mu_1)) - 1)^{-1} |\langle \mathbf{e}_k^R, u \rangle|^2 \\ &\leq R^{-3} (\exp(\beta(\frac{\varepsilon_0^1 - C}{R^2})) - 1)^{-1} |\langle \mathbf{e}_k^1(R^{-1}x), u(x) \rangle|^2 \end{aligned}$$

(B) is used in these estimates.

Since obviously

$$R^{-3} (\exp(\beta(\frac{\varepsilon_0^1 - C}{R^2})) - 1)^{-1} \xrightarrow{R \rightarrow \infty} 0$$

and

$$| \langle e_k^1(R^{-1}x), u(x) \rangle |^2 \xrightarrow{R \rightarrow \infty} | e_k^1(0) \widehat{u}(0) |^2,$$

so from $(u, u)_R$ in the limit $R \rightarrow \infty$ only remains the series

$$\begin{aligned} \sum_{k=L}^{\infty} (\exp(\beta(\varepsilon_k^R - \mu_2)) - 1)^{-1} | \langle e_k^R, u \rangle |^2 &= \\ &= z_2 (1 - z_2)^{-1} R^{-3-2l} \left| \int_{\Lambda_R} \overline{Q(x)} u(x) dx \right|^2 \\ &\quad (\text{ } \hat{\text{z}}(B) \text{ and } e_L^1 = Q \text{ homogeneous of degree } l) \\ &\quad + \sum_{k=L+1}^{\infty} z_2 (e^{\beta \varepsilon_k^R} - z_2)^{-1} | \langle e_k^R, u \rangle |^2, \end{aligned} \quad (F)$$

with $z_2 = e^{\beta \mu_2}$.

From (CON) follows that $z_2(1 - z_2)^{-1} R^{-3-2l}$ tends towards c for $R \rightarrow \infty$, and Lemma 5.1.3 ensures that the last row for $R \rightarrow \infty$ tends towards $\langle w_\zeta * u, u \rangle$

To justify this, note that in the series

$$\sum_{n=1}^{\infty} z_2^n K_R(n\beta) = \sum_{n=1}^{\infty} \sum_{k=L+1}^{\infty} z_2^n e^{-n\beta \varepsilon_k^R} | \langle e_k^R, u \rangle |^2$$

the summation over n and k can be interchanged thanks to the asymptotic behavior of the eigenvalues (see Theorem A.5, p. 64).

With this is proved that

$$\lim_{R \rightarrow \infty} (u, u)_R = c \left| \int_{\mathbb{R}^3} \overline{Q} u dx \right|^2 + \langle w_\zeta * u, u \rangle$$

which yields (1) of the Main Theorem.

The proof of (3) is completely analogous with

$$\begin{aligned} n_V(R) &= \sum_{k=0}^{L-1} (\exp(\beta(\varepsilon_k^R - \mu_1)) - 1)^{-1} \int_V |e_k^R(x)|^2 dx + \\ &\quad + \sum_{k=L}^{\infty} (\exp(\beta(\varepsilon_k^R - \mu_2)) - 1)^{-1} \int_V |e_k^R(x)|^2 dx \end{aligned}$$

and using Lemma 5.1.4.

The statement (2) of Theorem 5.1.2. follows directly from Lemma 2.2.1. and (2) in Theorem 3.3.2. □

Below we will specify in mor detail the relationship between the kinetic energy density $\frac{c}{2} \|\text{grad } Q\|^2$ in the condensate (viz. (4.2.6) with $q = \sqrt{c} Q$) and the potential surface energy (cf. p. 43) of the state that is macroscopically occupied in the thermodynamic limit.

The preconditions of Theorem (5.1.2.) shall still apply, in particular the boundary conditions (5.1.1) for h in $\mathcal{H}$, see (5.1.2).

So we agree upon

$$\partial \phi = p \phi$$

with $p = Q^{-1} \partial Q$ on the boundary $\partial \Lambda_R$.

Let q be the quadratic form on $\mathcal{H}$ with boundary potential $p = Q^{-1} \partial Q$ on $\partial \Lambda_R$ as on page 41. For every state $u \in \mathcal{H} = L^2(\Lambda_R)$, $u \in H_1(\Lambda_R)$ (see Appendix), $q(u)$ is the expected value of the potential surface energy of the state u .

The contribution of all particles with wave function u to the potential surface energy of the Bose system in Λ_R is then, in any state ω_R , cf. (5.1.3),

$$\mathcal{O}(u) = \omega_R(N([u])q(u),$$

where $N([u])$ denotes the counter of particles in the state u , cf. 16.)

The following applies

Theorem 5.1.5. If e is the eigenstate e_L^R of h in $\mathcal{H}$, then

$$\lim_{R \rightarrow \infty} (\mathcal{O}(e))^{-1} c \int_{\Lambda_R} \|\text{grad } Q\|^2 dx = 1.$$

Proof

With the designations on page 48 holds

$$e = e_L^R(x) = R^{-\frac{3}{2}} Q(R^{-1}x) = R^{-\frac{3}{2}-l} Q(x).$$

Therefore

$$\omega_R(N([e])q(e) = \frac{z_2}{2(1-z_2)} \int_{\partial \Lambda_R} p \bar{e} e dS = \frac{z_2 R^{-R-2l}}{(1-z_2)} \int_{\partial \Lambda_R} \bar{Q} \partial Q \cdot dS.$$

↑ see (*), p. 41

Hence, with Green's first identity

$$\int_{\Lambda} u \Delta v dx = \int_{\partial \Lambda} u \partial v \cdot dS - \int_{\Lambda} \text{grad } u \cdot \text{grad } v dx,$$

in which the integral on the left obviously vanishes with $\Delta v = \Delta Q = 0$.

We thus get finally

$$\omega_R(N([e])q(e) = \frac{z_2}{2(1-z_2)} R^{-3-2l} \int_{\Lambda_R} \|\text{grad } Q\|^2 dx.$$

Now the assertion follows from (CON). □

Loosely speaking, Theorem 5.1.5 can be summarized by stating

Conclusion In the thermodynamic limit, the kinetic energy of the superflow is in equilibrium with its potential energy at the system boundary.

5.2. Bogoliubov's Method

The extremal KMS states of the free Bose system can be generated in a very simple and elegant way in the volume limit by perturbing the Hamiltonian in Λ_R with a source term. This additional term violates gauge invariance, indicating the presence of particle sources and sinks in the corresponding Gibbs state. (Remember the similar 'pull effect' of an attractive surface potential - represented in the previous section by the boundary conditions for the Laplacian and the 'broken' chemical potential $\mu = \mu(N, P)$.) In the limit $R \rightarrow \infty$ the perturbation of the Hamiltonian is reduced, but leaves its effect in the equilibrium state of the infinitely extended system.

I would like to thank Professor ROEPSTORFF for bringing this method to my attention, which was first introduced by BOGOLIUBOV [48] into quantum statistical mechanics as the so-called method of *quasi means*.

This proposed approach works as follows.

For a compact volume $\Lambda \subset \mathbb{R}^3$ with a sufficiently smooth surface $\partial\Lambda$ and again

$$\Lambda_R := \{x \in \mathbb{R}^3 \mid R^{-1}x \in \Lambda\}$$

(the conditions for Λ given on p. 41, f. may apply), let Δ be subject to boundary conditions

$$\partial\phi = p_R\phi \tag{5.2.1}$$

with a differentiable function $p_R(x) = R^{-1}p_1(R^{-1}x)$ defined on $\partial\Lambda_R$. (In contrast to Section 5.1., the boundary conditions (5.2.1) here only serve to ensure the self-adjointness and the asymptotic behavior of the spectrum of $-\Delta$ (as specified in Theorem A.5, p. 64) and is otherwise completely uncritical. Periodic boundary conditions in a cube would likewise be suitable here.)

Let the chemical potential $\mu = \mu(R) \mathbf{1}_{\mathcal{H}}$ of the one-particle Hamiltonian

$$h = -\frac{1}{2}\Delta - \mu \tag{5.2.2}$$

in $\mathcal{H} = L^2(\Lambda_R)$ satisfy

$$R^2\mu \leq C < \varepsilon_0^1, \tag{5.2.3}$$

where ε_0^1 denotes the smallest eigenvalue of $-\frac{1}{2}\Delta$ in $\mathcal{H}$.

From (5.2.3) it follows that h is always positive and with $z = e^{\beta\mu}$ applies

$$\lim_{R \rightarrow \infty} z (e^{\beta\varepsilon_0^R} - 1)^{-1} R^{-3} = 0. \tag{5.2.4}$$

Let $W_{\mathcal{F}}$ denote the Fock representation of the Weyl algebra over $\mathcal{H}$ in the symmetric Fock space $\mathcal{F}(\mathcal{H})$ and H the second quantization of h in $\mathcal{F}(\mathcal{H})$. Let Q be a Maxwell polynomial and H' be the operator

$$H' = W_{\mathcal{F}}(Q)^* H W_{\mathcal{F}}(Q). \tag{11} \tag{5.2.5}$$

Bogoliubov's approach can then be sketchily outlined in this way. If $A(u)$ is the self-adjoint generator of the unitary one-parameter group $W_{\mathcal{F}}(tu)$,

¹¹ Here we write shortly $W_{\mathcal{F}}(Q)$ instead of $W_{\mathcal{F}}(Q \upharpoonright \Lambda_R)$ and similarly $A(Q)$ instead of $A(Q \upharpoonright \Lambda_R)$.

then formally follows from

$$i[H, A(u)] = A(ihu)$$

first

$$\begin{aligned} [[H, iA(u)], iA(u)] &= \\ &= i[A(ihu), A(u)] = -\operatorname{Im} \langle ihu, u \rangle = \langle u, hu \rangle, \end{aligned}$$

and thus

$$\begin{aligned} W_{\mathcal{F}}(Q)^* H W_{\mathcal{F}}(Q) &= \\ &= H + [H, iA(Q)] + \frac{1}{2} [[H, iA(Q)], iA(Q)] \\ &= H + A(ihQ) + \frac{1}{2} \langle Q, hQ \rangle \\ &= H + \frac{1}{\sqrt{2}} a(ihQ) + \frac{1}{\sqrt{2}} a^*(ihQ) + \frac{1}{2} \langle Q, hQ \rangle \end{aligned}$$

The last line describes H' in the form used by Bogoliubov of an operator H perturbed by a source term. Since Q is a solution of the Laplace equation, the source term formally disappears when h in the limit $R \rightarrow \infty$ approaches the operator $-\frac{1}{2}\Delta$ in $L^2(\mathbb{R}^3)$ under the boundary conditions (5.2.1) and with the chemical potential (5.2.2), both vanishing for $R \rightarrow \infty$.

The mathematically sound definition of H' is (5.2.5). Since $W_{\mathcal{F}}(Q)$ is a unitary operator, i.e. $W_{\mathcal{F}}^*(Q) = W_{\mathcal{F}}^{-1}(Q) = W_{\mathcal{F}}(-Q)$, so H' is also self-adjoint and has the same spectrum as H . In particular, for H' there exists the Gibbs state ω'_R with generating functional $E'(R)$, which is represented in the symmetric Fock space by the density operator

$$\Gamma' = e^{-\beta H'} (\operatorname{Tr} e^{-\beta H'})^{-1} = W_{\mathcal{F}}^*(Q) \Gamma W_{\mathcal{F}}(Q),$$

with $\Gamma = e^{-\beta H} (\operatorname{Tr} e^{-\beta H})^{-1}$.

Main Theorem 5.2.1. (ROEPSTORFF)

- (1) If $\lim_{R \rightarrow \infty} \mu = 0$, then $E'(R)$ converges simply on $\mathcal{D}(\mathbb{R}^3)$ against the generating functional

$$E(u) = \exp(-i \operatorname{Im}(Q[u])) E_1(u), \quad u \in \mathcal{D}(\mathbb{R}^3),$$

of a state on the local Weyl algebra $\mathfrak{W}(\mathcal{D}(\mathbb{R}^3))$. [$E_1(u)$ as in (3.3.1), p. 26 (with $\zeta = 1$) and $Q[u]$ again denotes the distribution

$$u \longmapsto \int_{\mathbb{R}^3} \overline{Q} u \, dx \quad . \quad]$$

Main Theorem 5.2.1.**(cont'd)**

- (2) The state defined in (1) by the generating functional E extends continuously in the sense of Lemma 2.2.1. (i.e., by extending the associated cyclic representation, see p. 13) to a state ω on the tempered Weyl algebra $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$. Furthermore, ω is an extremal KMS state at inverse temperature β (also referred to as a β -KMS state) with respect to the free dynamics α with chemical potential $\mu = 0$ and the two-point function of ω is

$$\mathcal{W}(x, y) = \frac{1}{2} \overline{Q(x)} Q(y) + w_1(x - y),$$

Proof *Ad (1):*

$$\begin{aligned} E'(R)(u) &= \omega'_R(W(u)) = \text{Tr } \Gamma' W_{\mathcal{F}}(u) \\ &= \text{Tr } W_{\mathcal{F}}(Q)^* \Gamma W_{\mathcal{F}}(Q) W_{\mathcal{F}}(u) \\ &= \text{Tr } \Gamma W_{\mathcal{F}}(Q) W_{\mathcal{F}}(u) W_{\mathcal{F}}(-Q) \\ &= \text{Tr } (W_{\mathcal{F}}(Q)^* = W_{\mathcal{F}}(-Q)^\dagger) \\ &= \exp(-i \text{Im} \langle Q, u \rangle) E^R(u), \\ &\quad (\text{cf. (WR), p. 11}^\dagger) \end{aligned}$$

where

$$E^R(u) = \exp\left(-\frac{1}{4} \langle u, \coth\left(\frac{\beta h}{2} u\right) \rangle\right) \quad \text{cf. (5.1.4)}$$

is the generating functional of the grand canonical state with density operator Γ .

From $\lim_{R \rightarrow \infty} \mu = 0$, i.e. $\lim_{R \rightarrow \infty} z = 1$ for $z = e^{\beta \mu}$, and (5.2.3) it follows completely analogous to the proof of Theorem 5.1.2. that for all $u \in \mathcal{D}(\mathbb{R}^3)$ holds

$$\lim_{R \rightarrow \infty} E^R(u) = \exp\left(-\frac{1}{4} \|u\|^2 - \frac{1}{2} \langle w_1 * u, u \rangle\right) = E_1(u).$$

This completes the proof of (1).

Ad (2): Immediate consequence of Lemma 2.2.1. and Theorem 3.3.2.(note that $-i \text{Im}(Q[u]) = i \text{Re}(-i Q[u])$).

□

5.3. The Rotating Vessel

In experiments with superfluid helium, a whole series of critical phenomena are observed. For example, it is well known that helium II cannot be transported through capillaries at any speed (e.g. DAUNT and MENDELSSOHN [49], ALLEN and MISENER [50]). The transport speeds at which a pressure difference is first necessary to maintain the flow depend, among other things, on the vessel geometry and are generally higher the narrower the capillary is. A first explanation for these transport phenomena, which are still only incompletely understood, was already provided by

BIJL, DE BOER and MICHELS [51] in 1941. They describe the dependence of this so-called *critical velocity* v_{cr} near absolute zero temperature approximately by

$$v_{cr} = 2\pi\hbar / md ,$$

where m is the mass of the He atom and d the diameter of the capillary. So, when observing critical velocities, Planck's constant comes into play. Here again we have a macroscopic effect that, like vortex quantization, points directly to the quantum nature of the superfluid.

FEYNMAN [25] suggested that the occurrence of critical velocities in helium II is linked to phase transitions in the Bose gas, similar to those we described for the free Bose condensate. He explains the apparently sudden onset of viscosity in the superfluid transported through the capillary with the formation of quantized vortices (which, however, are not considered stable, but are supposed to dissipate into heat over time, cf. [25], p. 45). This lead to the assumption that critical transport velocities have something to do with the transfer of angular momentum from the vessel walls to the particles or clusters of the moving superfluid. The critical transport velocities would then be closely related to the critical *rotation* velocities observed in 1969 by PACKARD and SANDERS [16] in a rotating cylinder containing helium II.

For the special dynamics of the ideal Bose gas in a rotating reference system, BLUTT and BUTLER [12] used approximate methods to determine critical surface velocities of rotation at which the total angular momentum of the fluid in a cylindrical vessel increases suddenly. LEWIS and PULÉ [7] can claim to have rigorously confirmed this result for the infinite free Bose gas by finding a critical value

$$\Omega_\infty := \lim_{R \rightarrow \infty} R^2 \Omega(R)$$

for the surface velocity of a cylinder with condensate rotating around its axis. Above this critical surface velocity and maintaining the average local particle density, the condensate appears to flow towards the boundary. R here again denotes a homothety factor for the initial volume Λ and $\Omega(R)$ is the angular velocity of the system in Λ_R , see below.

In order to describe the approach in [7] in detail - and later later to suitably modify and even generalize it, we consider the cylinders

$$\Lambda_R := \{x \in \mathbb{R}^3 \mid R^{-1}x \in \Lambda\} \tag{5.3.1}$$

with

$$\Lambda := \{x \in \mathbb{R}^3 \mid x_1^2 + x_2^2 \leq a^2 \text{ and } |x_3| \leq (2\pi a^2)^{-1}\} , \tag{5.3.2}$$

where a is a fixed positive constant. In $\mathcal{H} := L^2(\Lambda_R)$ the Laplace operator with von Neumann boundary conditions¹² is defined as a self-adjoint operator in $\mathcal{H}$ and $-\frac{1}{2}\Delta$ exhibits the asymptotic behavior of the eigenvalues described in Appendix A.5.

¹² That is, $\partial\phi = 0$ on $\partial\Lambda_R$.

The one-particle Hamiltonian of the system rotating in the cylinder Λ_R around the z-axis with angular momentum $\Omega(R)$ is defined as

$$h := -\frac{1}{2}\Delta - \Omega(R)L_3 - \mu(R)\mathbf{1}_{\mathcal{H}}, \quad (5.3.3)$$

L_3 denoting the operator of the angular momentum around the cylinder axis.

The ground state e_0^R of h obviously depends on Ω .

Since for

$$\Omega(R) = R^{-2}\Omega(1)$$

clearly holds

$$e_0^R(x) = R^{-\frac{3}{2}} e_0^1(R^{-1}x)$$

and because $\mu(R)$ only causes a shift in the spectrum of h , it is sufficient to calculate the ground state for $R = 1$ and an arbitrary $\Omega(1)$ to determine the state e_0^R . This is what LEWIS and PULÉ did in [7]:

For $m \in \mathbb{Z}$, let C_m denote the first positive zero of $\frac{d}{dy} J_{|m|}$ (the derivative of the standard Bessel function $J_{|m|}$). Then for

$$\Omega(1) \in (\Omega_m, \Omega_{m+1}) \quad \text{with} \quad \Omega_m := (2a^2)^{-1}(C_m^2 - C_{m-1}^2)$$

the ground state of h for $R = 1$ is

$$e_0^1(r, \phi) = K_m J_{|m|}(C_m a^{-1}r) e^{im\phi}, \quad (5.3.4)$$

where we used cylinder coordinates, $r^2 = x_1^2 + x_2^2$.

The normalization factor K_m is given by

$$K_m = \sqrt{2} C_m (2\pi a^2 (C_m^2 - m^2) J_{|m|}(C_m))^{-1}.$$

The eigenvalue of the ground state of h for $\mu = 0$ and $\Omega \in (\Omega_m, \Omega_{m+1})$ is (still for $R = 1$)

$$\varepsilon_0^1 = (2a^2)^{-1} C_m^2 - \Omega m.$$

With suitable $\mu < 0$ it is ensured that h remains positive for all $R > 0$, so that in the Fock representation of the Weyl Algebra over $\mathcal{H} = L^2(\Lambda_R)$ the grand canonical state ω_R is well defined by the density operator

$$\Gamma = e^{-\beta H} (Tr e^{-\beta H})^{-1},$$

with H the second quantization of h .

The thermodynamic limit can then be carried out in various ways by appropriately controlling $\Omega(R)$ and $\mu(R)$. LEWIS and PULÉ [7] maintained the angular momentum density and the average particle density in Λ_R constant in the limit. This leads to a classical translation-invariant and isotropic Bose condensate. However, for $\Omega_\infty > \Omega_1$ the long range order parameter disappears in the two-point function ('the condensate moves to the boundary').

We now modify the procedure by requiring only convergence of the average particle density in a given compact volume. With a well-defined behavior of $\Omega(R)$ in the volume limit $R \rightarrow \infty$, certain equilibrium states occurring in this limit exhibit vortices with quantized circulation, the strength of which depends on the asymptotic value of $R^2 \Omega(R)$. Proceeding in this way, the Ω_m introduced above appear explicitly as critical values at which a phase transition occurs.

We assume that

$$\lim_{R \rightarrow \infty} R^2 \Omega(R) = \Omega \in \mathbb{R} \quad (5.3.5)$$

and for every bounded region $\mathcal{V} \subset \mathbb{R}^3$ with volume $V > 0$ the mean particle number $n_{\mathcal{V}}(R) = \sum_{k=0}^{\infty} (e^{\beta(\varepsilon_k^R - \mu(R))} - 1)^{-1} \int_{\mathcal{V}} |e_k^R(x)|^2 dx$ of the state ω_R reduced to $\mathcal{V}$ exists, as well as also the limit

$$\lim_{R \rightarrow \infty} n_{\mathcal{V}}(R) = n_{\mathcal{V}} \in [0, \infty) \quad (5.3.6)$$

(so in the limit the *average particle density* in $\mathcal{V}$ becomes $\rho_{\mathcal{V}} = V^{-1}n_{\mathcal{V}}$).

Then the following holds.

Main Theorem 5.3.1.

For all $R > 0$ let the one-particle hamiltonian h , cf. (5.3.3), be strictly positive (which can always be realized with suitable $\mu(R) < 0$) and let (5.3.5) apply with $\Omega \in (\Omega_m, \Omega_{m+1})$.

- (1) If the chemical potential disappears in the limit $R \rightarrow \infty$ and the average particle density $\rho_{\mathcal{V}}$ exceeds the critical density

$$\rho_{cr} = (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(1)$$

(cf. (4.1.3), p. 32), then the generating functional E^R of ω_R converges simply on $\mathcal{D}(\mathbb{R}^3)$ against the generating functional

$$E(u) = \exp\left(-\frac{1}{2}c|Q[u]|^2\right) E_1(u) \quad , \quad u \in \mathcal{D}(\mathbb{R}^3)$$

with

$$Q = \begin{cases} (x_1 + ix_2)^m & \text{if } m \geq 0 \\ (x_1 - ix_2)^{|m|} & \text{if } m < 0 \end{cases}$$

and

$$c = V(\rho_{\mathcal{V}} - \rho_{cr}) \left(\int_{\mathcal{V}} |Q|^2 dx \right)^{-1} .$$

- (2) If $\lim_{R \rightarrow \infty} e^{\beta\mu(R)} = \zeta \in (0, 1)$, then E^R converges simply on $\mathcal{D}(\mathbb{R}^3)$ against E_{ζ} , cf. (3.3.1), and $\rho_{\mathcal{V}} = (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(\zeta)$, cf. (4.1.3).
- (3) The generating functional E , cf. (1), extends continuously in the sense of Lemma 2.2.1 to the functional of a state ω on the tempered Weyl algebra $\mathfrak{W}(\mathcal{S}(\mathbb{R}^3))$ and ω is β -KMS with respect to the free dynamics with $\mu = 0$.

According to (1), the generating functional E is Gaussian, cf. page 14. In particular, the state ω associated to E , cf. (3), is quasi free and gauge invariant according to Theorem 3.3.2. and ω has the two-point function

$$\mathcal{W}(x, y) = c \overline{Q(x)} Q(y) + w_1(x - y). \quad (5.3.7)$$

Proof Ad (1): Essentially the same ideas are used as in the proof of Theorem 5.1.2., the main points being based on the work of LEWIS and PULÉ (loc. cit.).

Let again

$$\{\varepsilon_k^R\}_{k=0,1,\dots}$$

be the ordered eigenvalue spectrum of h , cf. (5.3.3), enumerated with its multiplicities, and

$$\{e_k^R\}_{k=0,1,\dots}$$

a corresponding orthonormal basis in $\mathcal{H} = L^2(\Lambda_R)$.

First, the convergence of $R^2 \Omega(R)$ against $\Omega \in (\Omega_m, \Omega_{m+1})$ ensures the simple convergence on $\mathcal{D}(\mathbb{R}^3) \times \mathcal{D}(\mathbb{R}^3)$ of

$$\sum_{k=0}^{\infty} z (e^{\beta \varepsilon_k^R} - z)^{-1} \overline{e_k^R(x)} e_k^R(y)$$

against $w_1(x - y)$. This follows from [7], Lemma 3, which is analogous to Lemma 5.1.3., but with the Geens function of the equation

$$\frac{\partial}{\partial t} u + \frac{1}{2} \Delta u - \Omega L_3 u = 0$$

instead of the heat equation being used.

Analogously to Lemma 5.1.4, it is then shown that

$$\sum_{k=0}^{\infty} z (e^{\beta \varepsilon_k^R} - z)^{-1} \int_{\mathcal{V}} |e_k^R(x)|^2 dx$$

converges against $V \rho_{cr}$, where $\rho_{cr} = (2\pi\beta)^{-\frac{3}{2}} g_{\frac{3}{2}}(1) = w_1(0)$.

Because of (5.3.6) therefore

$$\lim_{R \rightarrow \infty} z (e^{\beta \varepsilon_0^R} - z)^{-1} \int_{\mathcal{V}} |e_0^R(x)|^2 dx = V(\rho_{\mathcal{V}} - \rho_{cr}). \quad (*)$$

Furthermore, for sufficiently large R , due to $\lim_{R \rightarrow \infty} R^2 \Omega(R) = \Omega \in (\Omega_m, \Omega_{m+1})$, the ground state of h is (in cylinder coordinates)

$$e_0^R(r, \phi) = R^{-\frac{3}{2}} K_m J_{|m|}(C_m(aR)^{-1}r) e^{im\phi},$$

see (5.3.4).

In the series expansion of e_0^R in Cartesian coordinates the highest order term in R is

$$R^{-\frac{3}{2}-|m|} K_m 2^{-|m|} (|m|!)^{-1} (C_m a^{-1})^{|m|} Q(x) .$$

This term dominates (remains) for $R \rightarrow \infty$.

Therefore and because of (*)

$$z (e^{\beta \varepsilon_0^R} - z)^{-1} R^{-3-2|m|} K_m^2 (2^{|m|} |m|!)^{-2} (C_m a^{-1})^{2|m|}$$

converges to c .

So it immediately follows for $u \in \mathcal{D}(\mathbb{R}^3)$ that

$$z (e^{\beta \varepsilon_0^R} - z)^{-1} | < e_0^R, u > |^2$$

converges to $c |Q[u]|^2$.

Ad (2): Trivial consequence of Lemma 3 in [7].

Ad (3): Lemma 2.2.1.

□

From the two-point function (5.3.7) we immediately calculate the following superflow

$$v_s = \operatorname{Im} (Q^{-1} \operatorname{grad} Q) = m \frac{(-x_2, x_1, 0)}{x_1^2 + x_2^2}$$

which explicitly shows a quantized vortex in the x_3 -axis of magnitude $2\pi m$.

So Theorem 5.3.1 states in summary that under the conditions mentioned, in particular the asymptotic behavior of the surface velocity

$$\lim_{R \rightarrow \infty} R^2 \Omega(R) = \Omega \in (\Omega_m, \Omega_{m+1})$$

condensation takes place into a β -KMS state with a quantized vortex of strength $2\pi m$ in the x_3 -axis, with $m \in \mathbb{Z}$. The values $R^{-2} \Omega_m$ thus prove to be critical angular velocities at which the Bose system in Λ_R undergoes phase transitions between states of vortex strength $2\pi(m-1)$ and $2\pi m$, $m \in \mathbb{Z}$. The free Bose gas therefore exhibits phase transitions during rotation that are similar to those known from experiment with helium II; cf. [16].



6. Pressure and Entropy

Apart from temperature and chemical potential, the thermodynamic state variables of the equilibrium states we investigated have so far been completely disregarded. In fact, the thermodynamics of the symmetry-breaking KMS states is identical to that of the well-known homogeneous and isotropic Bose condensate. It is trivial in the sense that the condensed component does not contribute to pressure and entropy. Since we started from grand canonical states in a finite volume in order to generate the equilibrium states of the infinite system in the thermodynamic limit, the *pressure* is the appropriate quantity that, together with temperature, particle density, and the density of the internal energy, completely describes the thermodynamics of the free Bose gas. Using the example of the states generated in Section 5.1, we show that the condensed fraction of the gas does not contribute to the pressure. The same applies to the entropy density.

In the grand canonical Gibbs state ω_R with the density operator

$$\Gamma = e^{-\beta H} (\text{Tr } e^{-\beta H})^{-1} ,$$

see (5.1.3), the classical state equation for the pressure p is

$$p = \frac{1}{\beta V} \log \mathfrak{Z} ,$$

where $\mathfrak{Z} = \mathfrak{Z}(z, V, T) = \sum_{k=0}^{\infty} \log(1 - z(k) e^{-\beta \varepsilon_k^R})$ is the grand canonical partition function in the state ω_R .

So the pressure is

$$p = -\frac{1}{\beta V} \sum_{k=0}^{\infty} \log(1 - z(k) e^{-\beta \varepsilon_k^R}) ,$$

with $z(k) = z_1 = e^{\beta \mu_1}$ for $k < L$ and $z(k) = z_2 = e^{\beta \mu_2}$ for $k \geq L$ with μ_1, μ_2 as on page 50.

In the thermodynamic limit $R \rightarrow \infty$ condensation takes place in the L -th level (see proof of Theorem 5.1.2., in particular the key point (F) on p. 51) which thus contributes with

$$p_L = -\frac{1}{\beta V} \log(1 - z_2)$$

to the pressure.

From (CON), p. 46 it follows for a certain $C_1 \in \mathbb{R}_+$

$$\lim_{R \rightarrow \infty} (1 - z_2)^{-1} R^{-3-2l} \leq C_1$$

and therefore

$$\begin{aligned} 0 &\leq \lim_{R \rightarrow \infty} -\frac{1}{\beta V} \log(1 - z_2) = \lim_{R \rightarrow \infty} (\beta \text{Vol}(\Lambda_R))^{-1} \log(1 - z_2)^{-1} \\ &\leq \lim_{R \rightarrow \infty} (\beta \text{Vol}(\Lambda))^{-1} R^{-3} \log(C_1 + (3 + 2l) \log R) = 0 , \end{aligned}$$

which means that the partial pressure of the condensate disappears in the thermodynamic limit.

It is just as easily verified that similar estimates apply to the entropy per volume

$$s = \frac{\partial}{\partial T} \frac{1}{\beta V} \log \mathfrak{Z} .$$

Therefore, the thermodynamics of even the superfluid phases of the free Bose gas remains trivial, which is perhaps not very surprising for this fascinating class of 'macroscopically occupied' quantum ground states.

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Appendix

We summarize here some mathematical facts that were used in various parts of our studies.

Theorem A.1. (FRIEDRICHS, STONE)

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces over $\mathbb{C}$ and $\mathcal{K}$ be dense as a subset of $\mathcal{H}$. Also let the inclusion

$$\iota : \mathcal{K} \hookrightarrow \mathcal{H}$$

be continuous in the Hilbert space topologies of $\mathcal{H}$ and $\mathcal{K}$.

Then there exists exactly one positive self-adjoint operator T in $\mathcal{H}$ with domain $D_T = \mathcal{K}$ which - as an operator on $\mathcal{K}$ - embeds the latter isometrically in $\mathcal{H}$.

T is even an isometric isomorphism from $\mathcal{K}$ to $\mathcal{H}$.

(See [52], Chapter I, 2.1. The theorem is a reformulation of classical results, cf. [47], section 124.)

Corollary A.2. (The self-adjoint operator of a semi-bounded quadratic form)

Let $\mathcal{H}$ be a Hilbert space and $q : D \rightarrow \mathbb{R}$ a semi-bounded quadratic form closed on $D \subset \mathcal{H}$ and densely defined in $\mathcal{H}$. Hence for a certain $c \in \mathbb{R}$ holds

$$q(u) \underset{(\leq)}{\geq} c \langle u, u \rangle, \quad u \in D,$$

($\langle \cdot, \cdot \rangle$ denotes the scalar product in $\mathcal{H}$).

Then, the positive quadratic form

$$\tilde{q}(u) := \underset{(-)}{+} q(u) + \underset{(+)}{(1 - c)} \langle u, u \rangle \geq \langle u, u \rangle$$

is closed on D and by polarization $\tilde{q}$ becomes the scalar product of a Hilbert space $\mathcal{K}_D := (D, \tilde{q})$ with topology finer than that of $\mathcal{H}$.

If T is the operator of this Hilbert space $\mathcal{K}_D$ in the sense of Theorem A.1., then with the sesquilinear form $(\cdot, \cdot)_q$ derived from q , the operator

$$S := \underset{(-)}{+} T^2 - \underset{(+)}{(1 - c)} \mathbf{1}_{\mathcal{K}_D}$$

satisfies

$$(u, v)_q = \langle u, Sv \rangle.$$

for all $u \in \mathcal{K}_D$ and v in the domain $D_S \subset \mathcal{K}_D$ of S .

S is called the operator of the quadratic form q .

For every $\mathcal{K}$ and $\mathcal{H}$ that satisfy the conditions of Theorem A.1., the operator T of the theorem allows us to construct the following 'continuous' chain (in the sense of continuous inclusions $(*)$ below)

$$\underline{\mathcal{K} \mathcal{H}_s}, \quad s \in [0, 1]$$

of so-called *intermediate Hilbert spaces* between $\mathcal{K}$ and $\mathcal{H}$. Precisely, for $s \in [0, 1]$ the space $\underline{\mathcal{K} \mathcal{H}_s}$ is defined as the Hilbert space whose underlying set is the domain of T^{1-s} and whose scalar product is given by

$$\langle T^{1-s} u, T^{1-s} v \rangle.$$

The corresponding norm $\|T^{1-s}(u)\|$ is equivalent to the norm of the graph of T^{1-s} , that is to

$$(\|u\|^2 + \|T^{1-s} u\|^2)^{\frac{1}{2}},$$

as immediately follows from the inequality

$$\|T^{1-s} u\|^2 \geq \|\iota\|^{-(1-s)} \|u\|.$$

$\|\iota\|$ denotes the operator norm of the inclusion $\iota : \mathcal{K} \hookrightarrow \mathcal{H}$, which according to Theorem A.1. was assumed to be continuous. The inequality follows from the spectral theorem, according to which $\|\iota\|^{-1}$ is a lower bound of the spectrum of T .

Then for all $s, t \in [0, 1]$ such that $s \leq t$, the following inclusions are continuous, with dense range

$$\mathcal{K} = \underline{\mathcal{K} \mathcal{H}_0} \hookrightarrow \underline{\mathcal{K} \mathcal{H}_s} \hookrightarrow \underline{\mathcal{K} \mathcal{H}_t} \hookrightarrow \underline{\mathcal{K} \mathcal{H}_1} = \mathcal{H} \quad (*)$$

(for more see [52]).

In boundary value problems with partial differential operators *Sobolev spaces* play an important role. With the Sobolev spaces defined below, we ensure that the Laplacian in a bordered finite volume Λ is well-defined as a self-adjoint operator in a Hilbert space of functions in Λ .

Definition (1) Let Σ be any n -dimensional borderless compact Riemannian manifold, Δ_Σ be the Laplace-Beltrami operator, self-adjoint in $L^2(\Sigma)$.

Define the Sobolev space $H_s(\Sigma)$ at index $s \in [0, \infty)$ as the following topological vector space¹³:

For $s = 2m$, $m \in \mathbb{N}$, **let** $H_s(\Sigma)$ be the space whose underlying set is the domain of Δ_Σ^m in $L^2(\Sigma)$ and whose topology is generated by the norm of the graph of Δ_Σ^m .

For $s = 2(m - \delta)$, $m \in \mathbb{N}_+$ **and** $\delta \in [0, 1]$, **let**

$$H_s(\Sigma) := \underline{H_{2m}(\Sigma) H_{2(m-1)}(\Sigma)_\delta}$$

¹³ According to the foregoing, the Sobolev spaces are actually intermediate Hilbert spaces, but we are not interested in any special metric here.

Definition (2) Let Λ be a n -dimensional bordered compact Riemann C^∞ submanifold of Σ , which lies entirely in the domain of a map. Then define:

$$H_s(\Lambda) := H_s(\Sigma) / N(\Lambda)$$

provided with the quotient topology.

Λ is identified here with its isometric image in Σ and $N \subset H_s(\Sigma)$ is the subspace of all $u \in H_s(\Sigma)$, such that $u|_\Lambda = 0$ almost everywhere.

The definition of $H_s(\Lambda)$ turns out to be independent of the manifold Σ that embeds Λ . In particular, (2) uniquely defines Sobolev spaces $H_s(\Lambda)$, $s \in [0, \infty)$ for bounded compact C^∞ submanifolds of $\mathbb{R}^n$, since each such Λ is embedded in a torus Σ .

Remark Note that for all $s, t \in [0, \infty)$ with $s \geq t$ $H_s(X)$ is dense in $H_t(X)$ with continuous inclusion, and $H_0(X) = L^2(X)$.

In the literature, Sobolev spaces are often defined using local coordinates (i.e. maps), see [52], for example. We like the definition above without maps for its elegance.

Theorem A.3 (Trace Theorem)

Let Λ be a n -dimensional compact C^∞ submanifold of $\mathbb{R}^n$ with smooth border $\partial\Lambda$ and ∂ be the inner normal derivative on $\partial\Lambda$. Furthermore, let $s \in \mathbb{R}_+$, $k, m \in \mathbb{N}$, $s > m + \frac{1}{2}$, $s \geq k$ and D^k be any k -th order partial differential operator.

(1) The mapping

$$\partial^m : \mathcal{D}(\Lambda) \longrightarrow \mathcal{D}(\partial\Lambda)$$

continuously extends to a linear continuous surjection from $H_s(\Lambda)$ to $H_{s-m-\frac{1}{2}}(\partial\Lambda)$.

(2) The derivative in the distribution sense

$$D^k : H_s(\Lambda) \longrightarrow H_{s-k}(\Lambda)$$

is continuous.

Proof: [52], (1) see Theorem 9.4., (2) see Theorem 9.7.

Theorem A.4 (The quadratic form of the Laplace operator)

Let the preconditions of Theorem A.3 apply and $\Lambda \subset \mathbb{R}^3$. Furthermore let p be a bounded real-valued measurable function on $\partial\Lambda$.

Then the quadratic form on $H_1(\Lambda)$

$$q(u) := - \int_{\Lambda} \|\text{grad } u\|^2 dx - \int_{\partial\Lambda} p |u|_{\circ}^2 dS$$

is upper bounded and closed in $H_1(\Lambda)$ with respect to $L^2(\Lambda)$.

($u|_{\circ}$ above denotes the continuation of u to $H_{\frac{1}{2}}(\partial\Lambda)$ according to Theorem A.3.(1).)

Proof: First, q is continuous on $H_1(\Lambda)$ by the Trace Theorem. It then follows from Sobolev's inequalities 16.4 and 16.5, cf. [53], p. 124, and from [52], Theorem 9.7. that with a certain $K \in \mathbb{R}_+$ in the quadratic form

$$\tilde{q}(u) := -q(u) + K \|u\|_{L^2(\Lambda)}^2$$

holds in the sense of norm equivalence, i.e.

$$q(u) \cong \|u\|_{H_1(\Lambda)}^2.$$

This implies the closedness of $\tilde{q}$ in $L^2(\Lambda)$, hence likewise the closedness of q , and also boundedness. □

Definition (The Laplacian with Boundary Conditions)

The preconditions of Theorem A.4. apply with $\Lambda \subset \mathbb{R}^3$.

The due to Corollary A.2 well-defined and unique self-adjoint operator in $L^2(\Lambda)$ associated to quadratic form q of Theorem A.4. is called the Laplacian with boundary conditions

$$\partial \phi = p \phi$$

Theorem A.5. (MIZOHATA, ARIMA [54])

Let Λ be a 3-dimensional compact C^∞ submanifold of $\mathbb{R}^3$ with a smooth boundary, $p \in \mathcal{D}(\partial \Lambda)$ real-valued, and Δ be the Laplace operator with boundary conditions

$$\partial \phi = p \phi \quad \text{on} \quad \partial \Lambda.$$

Furthermore, let $G(x, y, t)$ be the Greens function of the heat equation

$$\frac{\partial}{\partial t} u = -\Delta u$$

with the same boundary conditions and $G_F(x, y, t)$ be a fundamental solution of the heat equation in $\mathbb{R}^3 \times \mathbb{R}_+$. Finally let $G_C := G - G_F$.

Then the following holds

- (1) $-\Delta$ has a purely discrete spectrum, bounded from below and every eigenvalue has finite multiplicity.
- (2) If the spectrum of $-\Delta$ enumerated with its multiplicities is

$$\{\varepsilon_k\}_{k \in \mathbb{N}}$$

then a $C_1 \in \mathbb{R}_+$ exists, such that for almost all $k \in \mathbb{N}$ (i.e. up to a finite number) holds

$$\varepsilon_k \geq C_1 k^{\frac{1}{2}} \tag{A.5}$$

Theorem A.5. (MIZOHATA, ARIMA [54])
(cont'd)

- (3) Let an orthonormal system matching the spectrum $\{\varepsilon_k\}_{k \in \mathbb{N}}$ be given by

$$\{\mathbf{e}_k\}_{k \in \mathbb{N}} \text{ .}$$

Then there exists a positive konstant C_2 such that for almost all $k \in \mathbb{N}$ holds

$$\sup_{x \in \Lambda} |\mathbf{e}_k(x)| \leq C_2 \varepsilon_k \text{ .}$$

- (4) For every $t \in \mathbb{R}_+$ there exists a constant $c(t) \in \mathbb{R}_+$ such that for all $s \in \mathbb{R}_+$ with $s \leq t$

$$|G(x, y, s)| \leq \frac{c(t)}{s^{3/2}} \exp\left(-\frac{l_y^2}{2s}\right) \text{ ,}$$

where $l_y := \text{dist}(y, \partial\Lambda) = \inf_{z \in \partial\Lambda} \|y - z\|$.



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List of Symbols

$\mathfrak{A}$	C*-Algebra with unit	p. 11
α_t	Dynamical one-parameter group	p. 21
β	Inverse absolute temperature	p. 22
$\mathcal{B}(\mathcal{H})$	Algebra of bounded operators of a Hilbert space $\mathcal{H}$	p. 12
$\mathcal{D}(\Lambda)$	$\mathbb{C}$ -valued C^∞ functions with compact support in Λ	p. 12
E	Generating functional of any state	p. 12
$E_{\mathcal{F}}$	Fock functional	p. 14
E_ζ		p. 26
$\mathcal{F}(\mathcal{H})$	Symmetric Fock space over a Hilbert space $\mathcal{H}$	p. 15
Γ	Density operator of a grand canonical Gibbs state	p. 43
$H_s(X)$	Sobolev space	p. 11
$\dot{j}_s$	Particle current density	p. 18
$L^2(\Lambda)$	Hilbert space of square-integrable functions with domain $\Lambda \subset \mathbb{R}^3$	p. 14
$\mathcal{L}$	Symplectic space	p. 12
μ	Chemical potential	p. 26
$\boldsymbol{\mu}(P)$		p. 43
$N(M)$	Counter of particles in a finite dimensional (sub-)space M	p. 16
$\mathcal{N}$		p. 43
ω	Any state	p. 12
$\mathcal{P}$		p. 43
$\pi_{\mathcal{F}}$	Fock representation	p. 15
Q	Maxwell polynomial	p. 27
$Q[u]$		p. 27
ρ	Particle number density	p. 18
$\mathcal{S}(\mathbb{R}^n)$	Space of rapidly decaying $\mathbb{C}$ -valued C^∞ functions in $\mathbb{R}^n$	p. 12
$\mathcal{S}'(\mathbb{R}^n)$	Space of tempered distributions in $\mathbb{R}^n$ (dual space of $\mathcal{S}(\mathbb{R}^n)$)	p. 12
$\mathbf{v}_s$	Superflow velocity	p. 34
W	Weyl*system	p. 11
$\mathcal{W}(x, y)$	Two-point function	p. 15
$\mathfrak{W}(\mathcal{L})$	Weyl algebra over a prehilbert space $\mathcal{L}$	p. 11
w_ζ		p. 26
$\mathcal{Z}$	Space of Fourier transforms of $\mathcal{D}(\mathbb{R})$ analytically continued to $\mathbb{C}$	p. 23
ζ	Fugacity	p. 26

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